

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042816\
 Data File : BF086472.D
 Acq On : 28 Apr 2016 19:29
 Operator : UM/SJ
 Sample : H2702-08
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TEC-COMP-B1D

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-BF042716.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	2.201	7	10	19	rVB	407740	715262	13.70%	1.599%
2	4.967	249	252	260	rBV	112178	172882	3.31%	0.387%
3	5.378	285	288	291	rBV	3621826	4057265	77.71%	9.072%
4	6.430	376	380	382	rBV	3987485	5220805	100.00%	11.673%
5	6.556	388	391	393	rBV	4399979	4632165	88.73%	10.357%
6	6.784	409	411	421	rBV	1040711	1002246	19.20%	2.241%
7	6.944	422	425	427	rBV	3430760	3410433	65.32%	7.626%
8	7.356	458	461	463	rBV	2736848	3204986	61.39%	7.166%
9	7.447	467	469	477	rVB2	59500	130194	2.49%	0.291%
10	8.076	521	524	526	rBV	929828	1229717	23.55%	2.750%
11	8.190	532	534	542	rVB	35004	53992	1.03%	0.121%
12	8.613	568	571	573	rVB2	42756	58723	1.12%	0.131%
13	8.933	596	599	605	rBV2	66949	116268	2.23%	0.260%
14	9.150	615	618	621	rBV	4302378	4635287	88.78%	10.364%
15	9.550	650	653	655	rBV	584094	690208	13.22%	1.543%
16	9.825	674	677	679	rBV	1646676	1499917	28.73%	3.354%
17	10.259	712	715	717	rBV2	98593	163188	3.13%	0.365%
18	10.488	731	735	738	rBV	58639	108068	2.07%	0.242%
19	10.613	743	746	749	rBV	3028260	3309430	63.39%	7.400%
20	10.739	755	757	763	rVB	195610	283871	5.44%	0.635%
21	10.933	772	774	778	rBV2	27216	60946	1.17%	0.136%
22	11.185	794	796	797	rBV	124405	107238	2.05%	0.240%
23	11.299	804	806	809	rBV	913595	1351236	25.88%	3.021%
24	12.716	928	930	933	rBV	260758	256248	4.91%	0.573%
25	12.899	943	946	948	rBV	3687886	5002417	95.82%	11.185%
26	13.425	989	992	994	rBV	192190	185534	3.55%	0.415%
27	13.791	1021	1024	1032	rBV	168107	270095	5.17%	0.604%
28	13.928	1034	1036	1044	rVV	796554	1239914	23.75%	2.772%
29	14.111	1050	1052	1056	rVB	50062	57087	1.09%	0.128%
30	14.419	1077	1079	1081	rBV	45040	53565	1.03%	0.120%
31	14.694	1100	1103	1107	rBV2	243714	409152	7.84%	0.915%
32	14.774	1108	1110	1113	rVB	95456	136105	2.61%	0.304%
33	15.334	1156	1159	1162	rBV	640600	825029	15.80%	1.845%
34	19.083	1483	1487	1498	rVB3	17829	74516	1.43%	0.167%

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ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

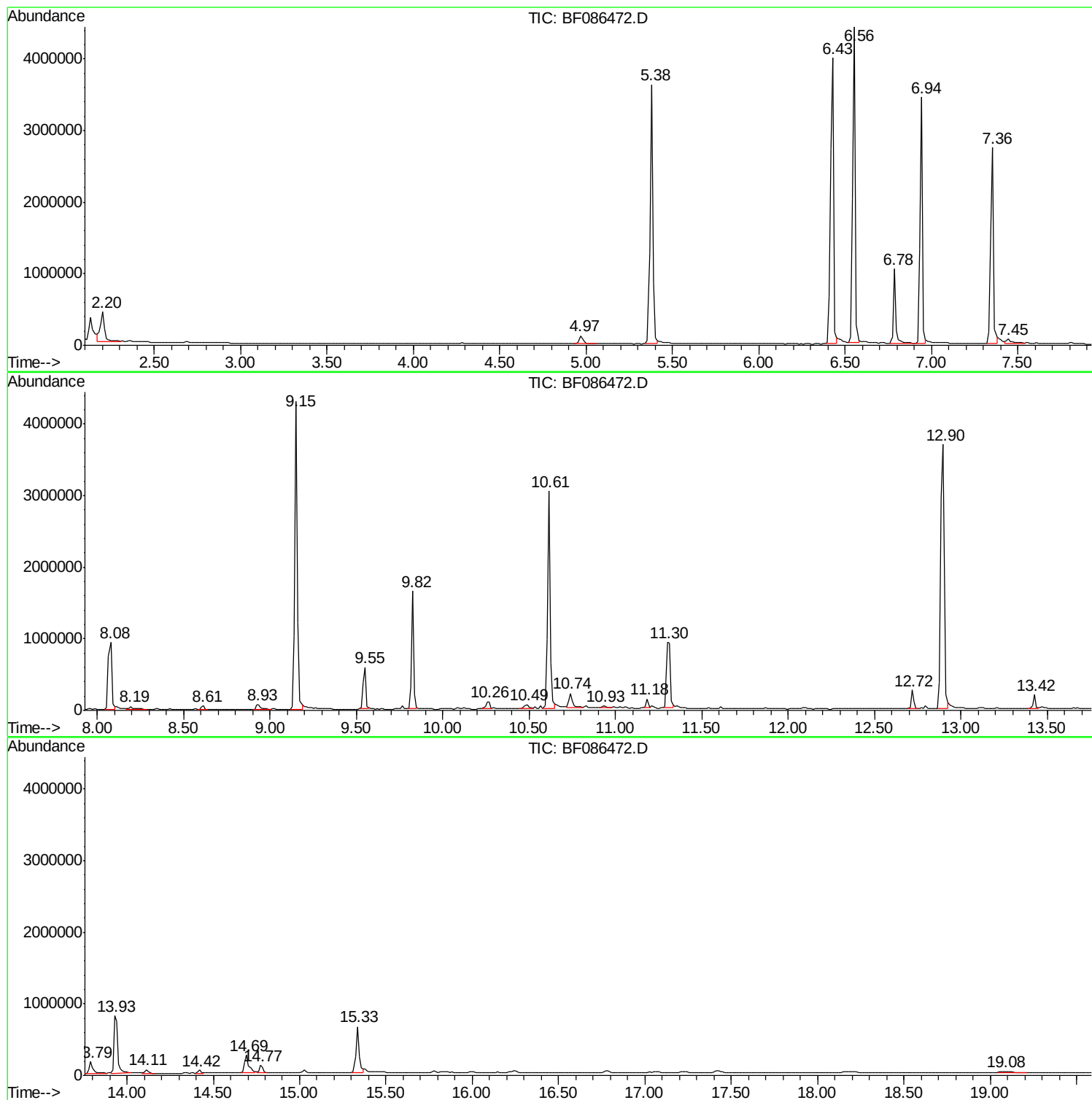
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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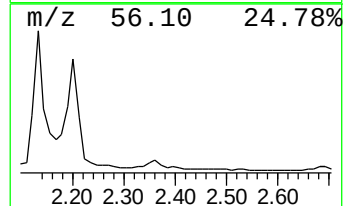
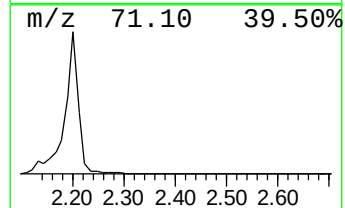
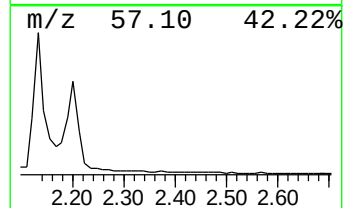
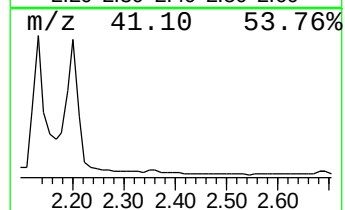
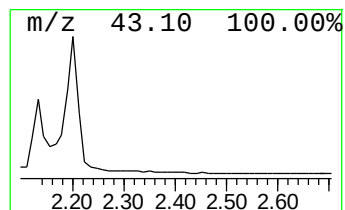
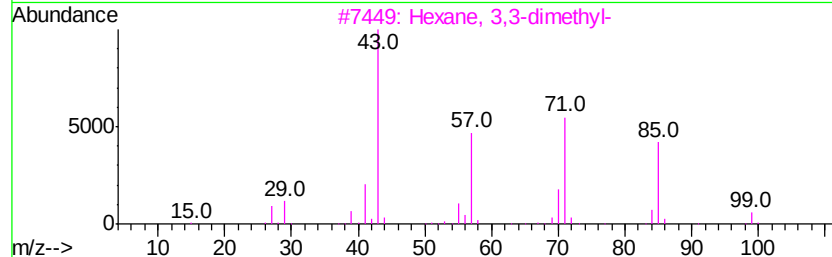
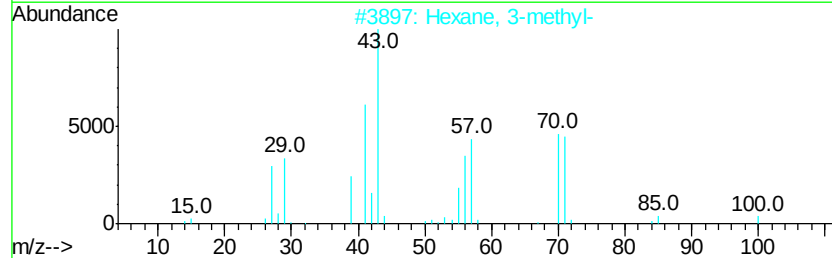
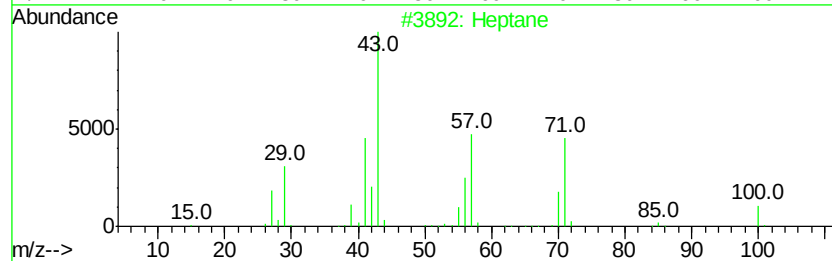
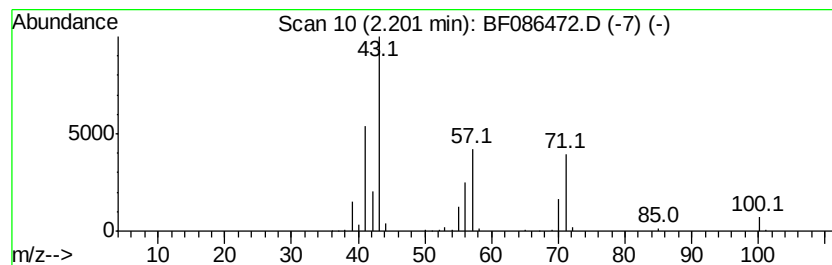
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Heptane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.20	14.27 ng	715262	1,4-Dichlorobenzene-d4	6.78

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane		100	C7H16	000142-82-5	91
2	Hexane, 3-methyl-		100	C7H16	000589-34-4	50
3	Hexane, 3,3-dimethyl-		114	C8H18	000563-16-6	47
4	1-Pentanol, 2-methyl-		102	C6H14O	000105-30-6	39
5	Hexane, 2,3-dimethyl-		114	C8H18	000584-94-1	38



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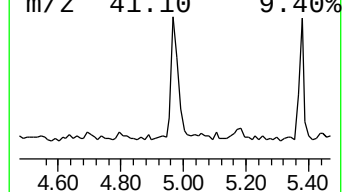
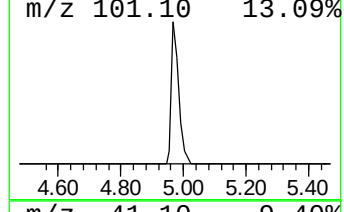
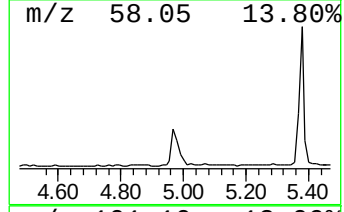
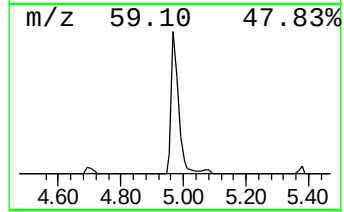
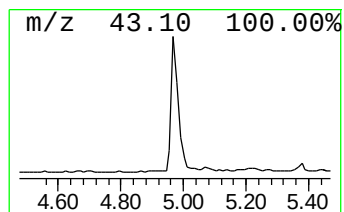
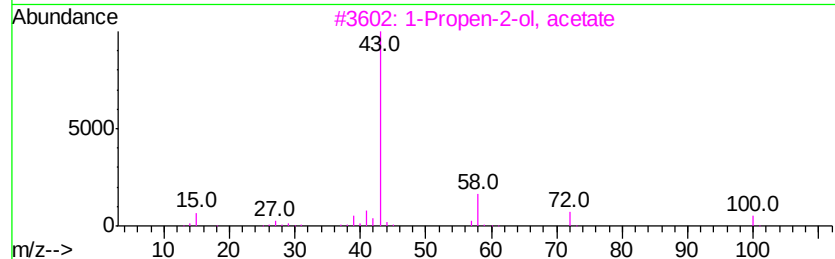
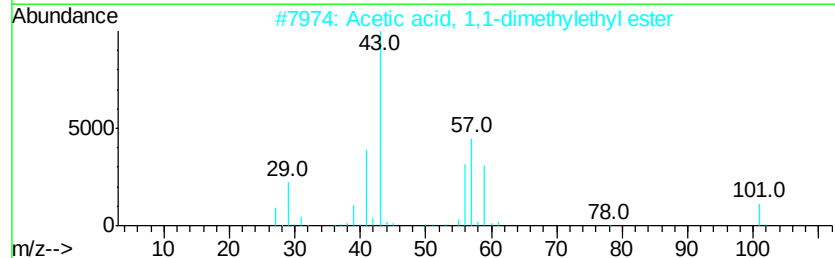
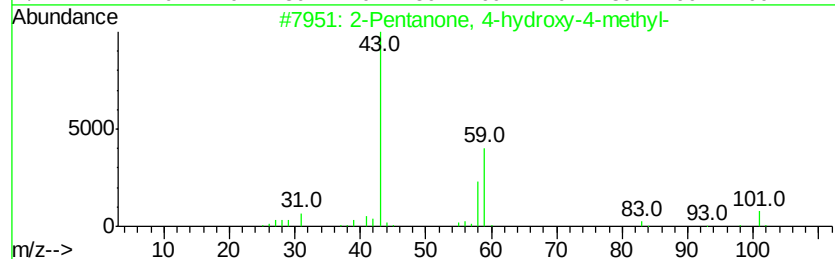
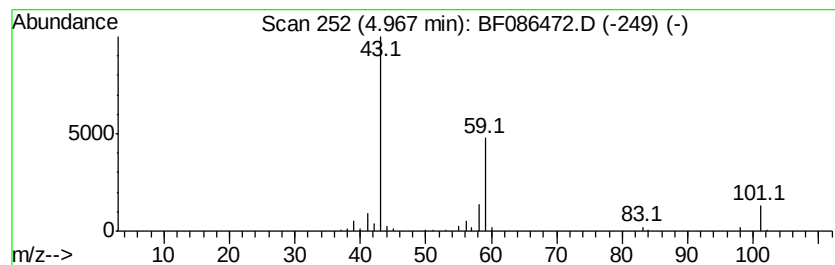
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	3.45 ng	172882	1,4-Dichlorobenzene-d4	6.78

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Butane	58	C4H10	000106-97-8	9



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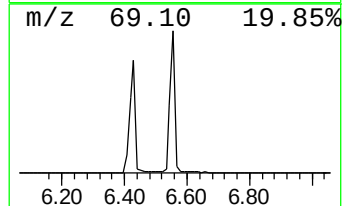
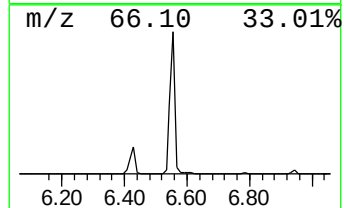
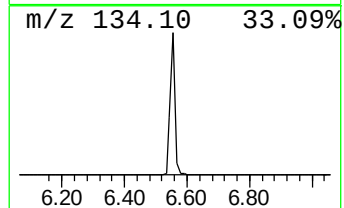
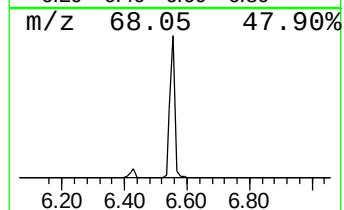
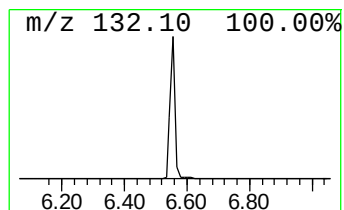
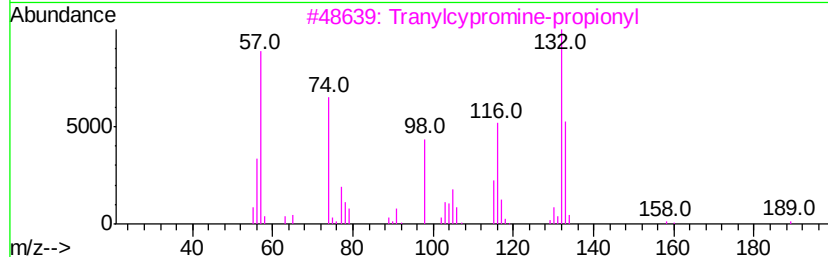
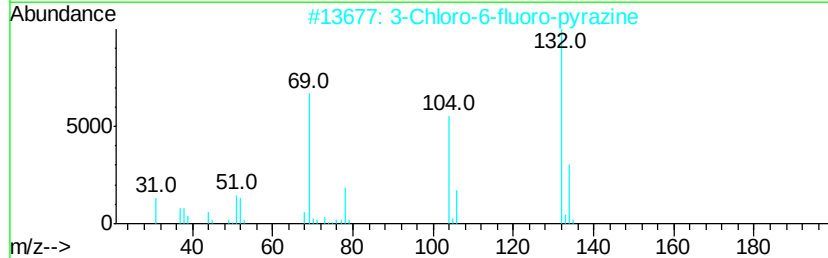
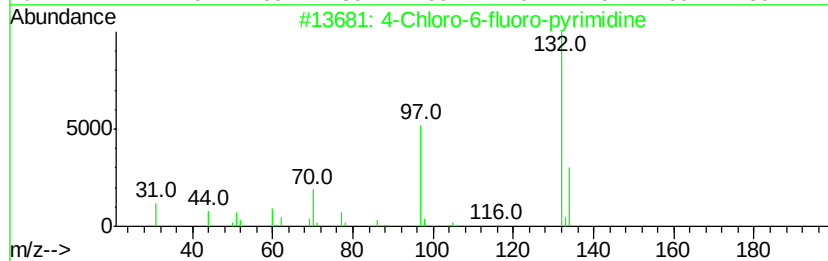
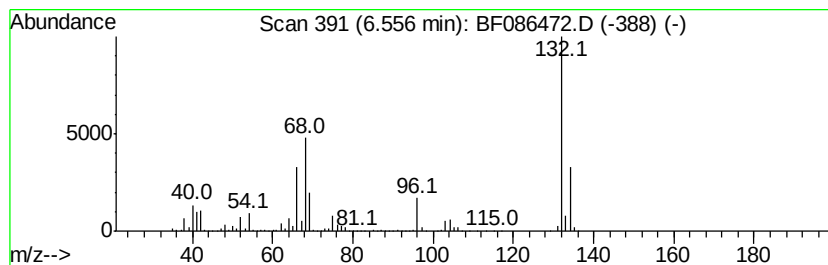
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	92.44 ng	4632170	1,4-Dichlorobenzene-d4	6.78

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		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	22
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16



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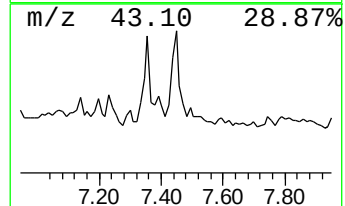
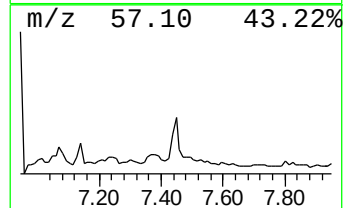
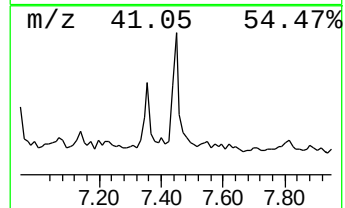
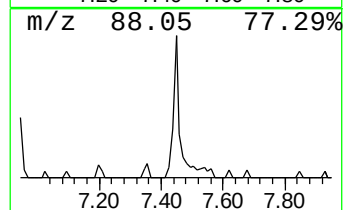
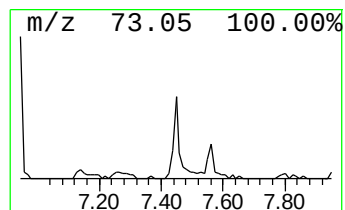
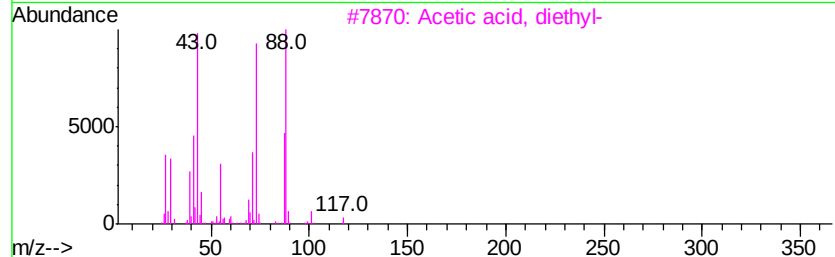
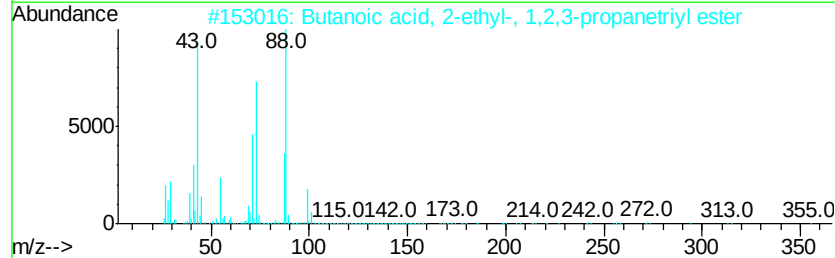
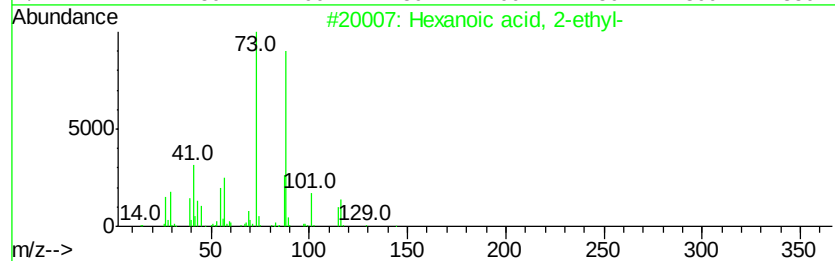
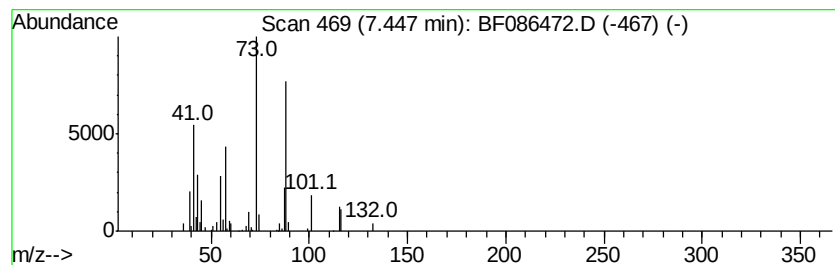
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Hexanoic acid, 2-ethyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.45	2.12 ng	130194	Naphthalene-d8	8.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	83
2		Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	42
3		Acetic acid, diethyl-	116	C6H12O2	000088-09-5	40
4		Propanoic acid, 3-hydroxy-2-meth...	118	C5H10O3	042998-03-8	40
5		Hydroxypivalic acid	118	C5H10O3	004835-90-9	38



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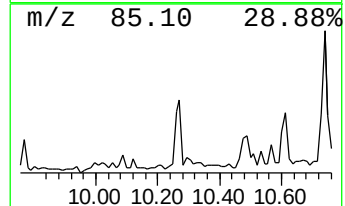
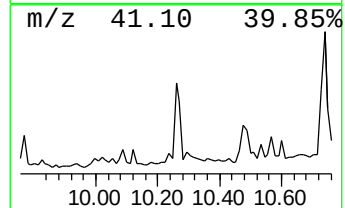
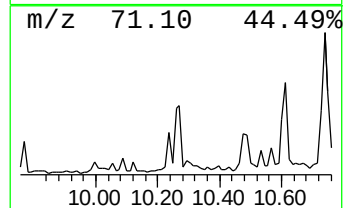
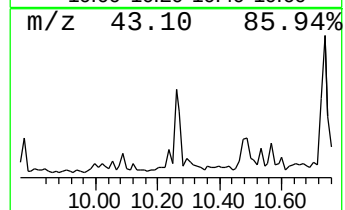
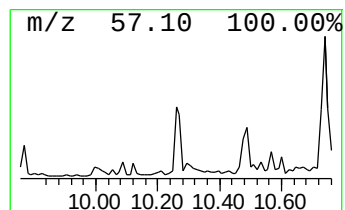
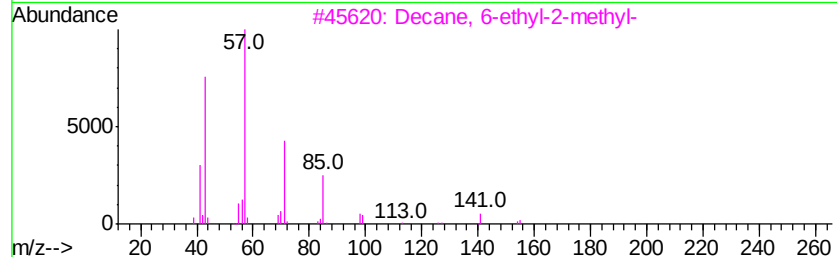
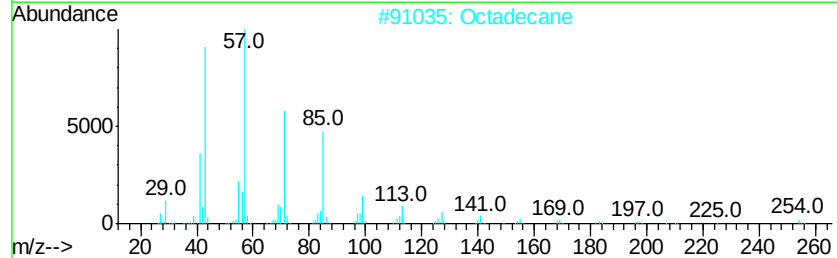
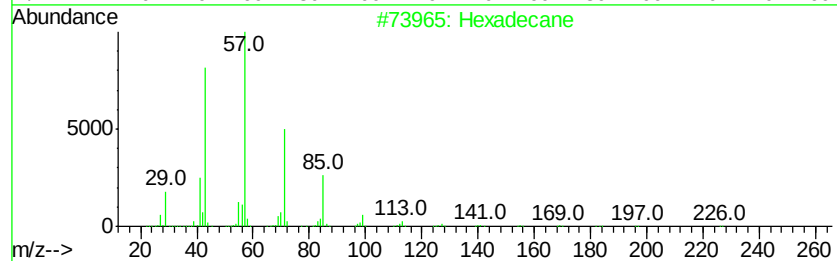
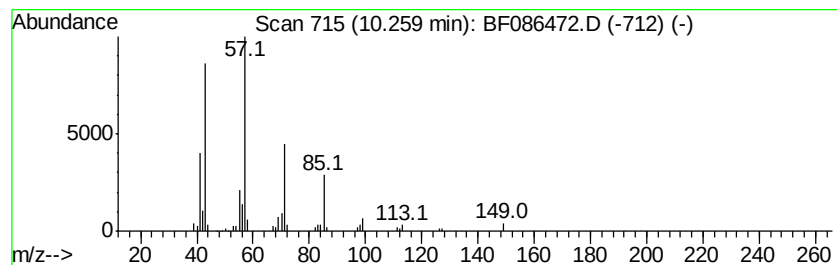
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hexadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.26	2.18 ng	163188	Acenaphthene-d10		9.82
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Octadecane	254	C18H38	000593-45-3	86
3	Decane, 6-ethyl-2-methyl-	184	C13H28	062108-21-8	78
4	Heptadecane	240	C17H36	000629-78-7	64
5	Heptadecane, 2,6,10,14-tetramethyl-	296	C21H44	018344-37-1	59



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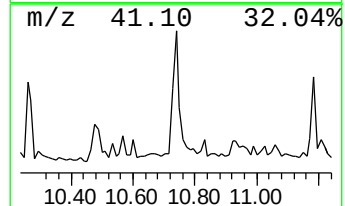
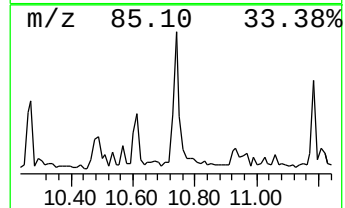
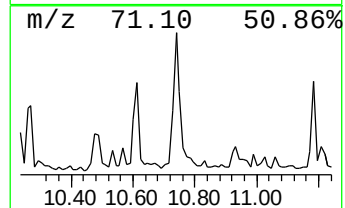
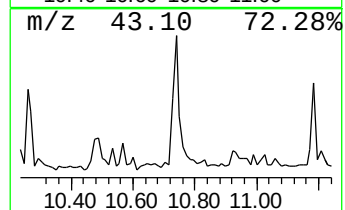
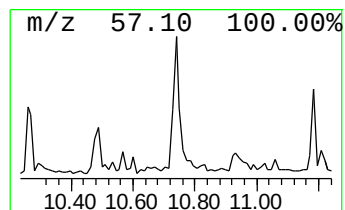
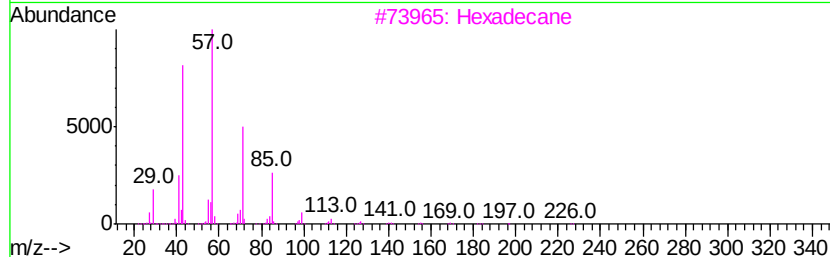
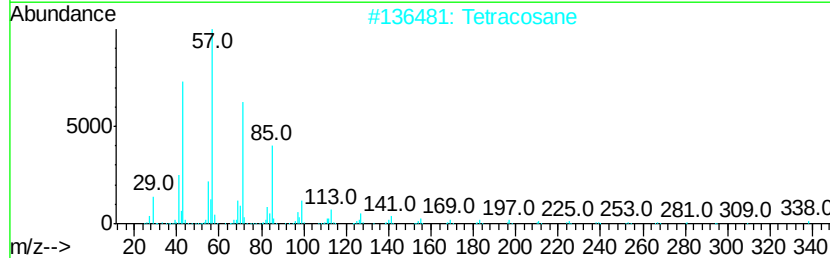
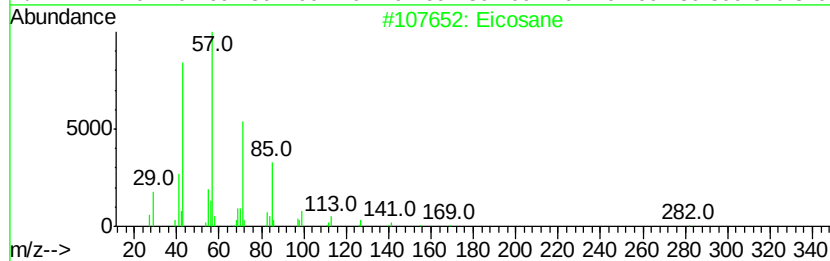
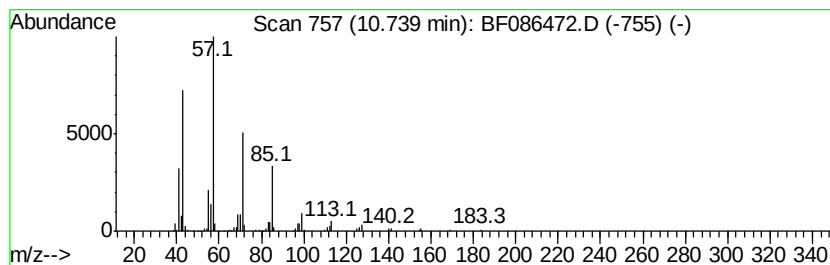
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ClientSampleId :
TEC-COMP-B1D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.74	4.20 ng	283871	Phenanthrene-d10		11.31
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Tetracosane	338	C24H50	000646-31-1	90
3	Hexadecane	226	C16H34	000544-76-3	90
4	Heptadecane	240	C17H36	000629-78-7	86
5	Tetradecane	198	C14H30	000629-59-4	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042816\
Data File : BF086472.D
Acq On : 28 Apr 2016 19:29
Operator : UM/SJ
Sample : H2702-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

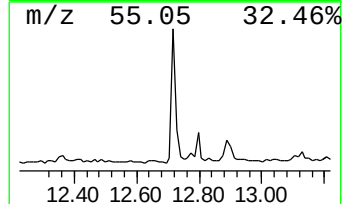
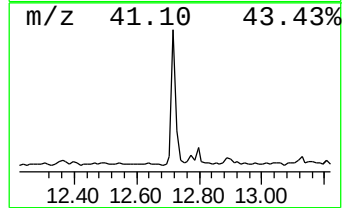
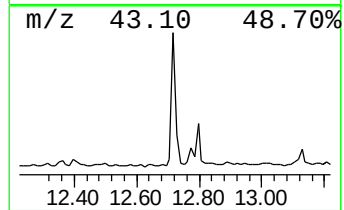
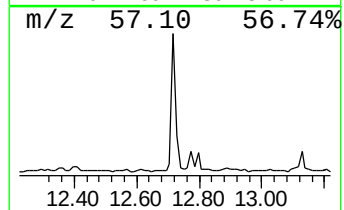
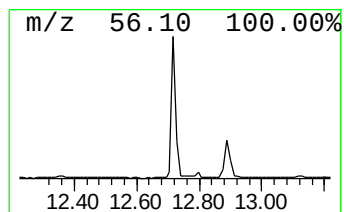
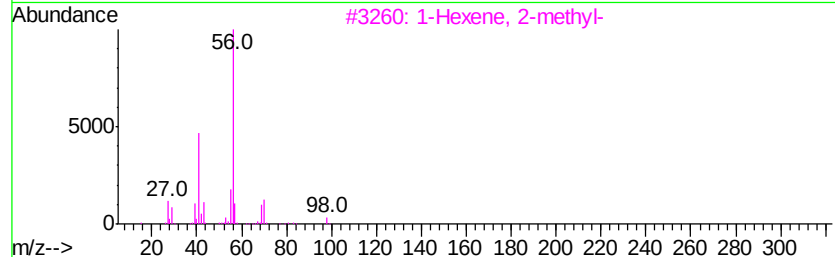
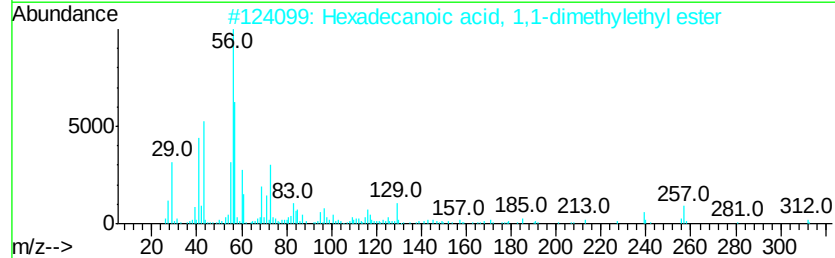
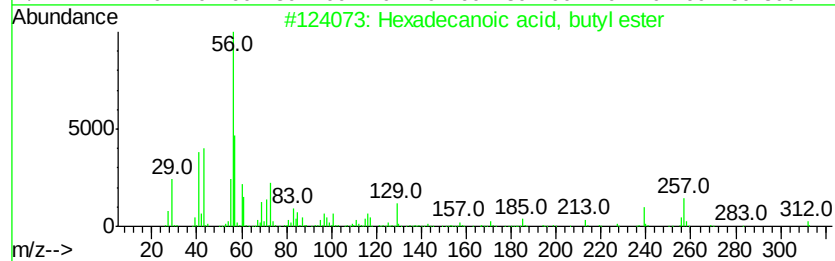
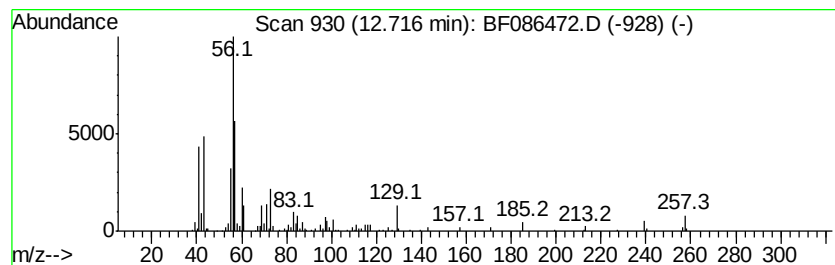
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ClientSampleId :
TEC-COMP-B1D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.72	4.13 ng	256248	Chrysene-d12		13.94
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	53
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	53
3	1-Hexene, 2-methyl-	98	C7H14	006094-02-6	38
4	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	38
5	Cyclopentanone, 2,2-dimethyl-	112	C7H12O	004541-32-6	38



Data Path : Z:\HPCHEM1\BNA F\DATA\BF042816\
Data File : BF086472.D
Acq On : 28 Apr 2016 19:29
Operator : UM/SJ
Sample : H2702-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TEC-COMP-B1D

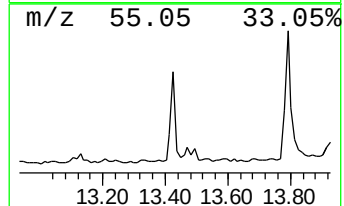
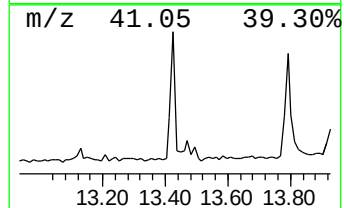
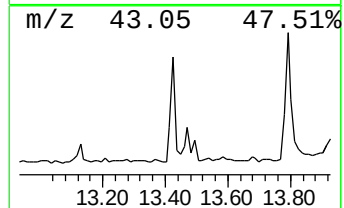
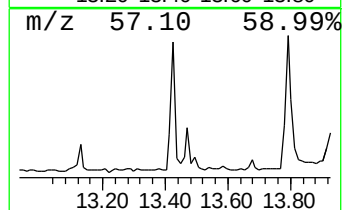
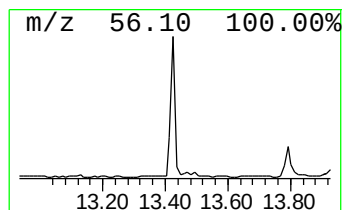
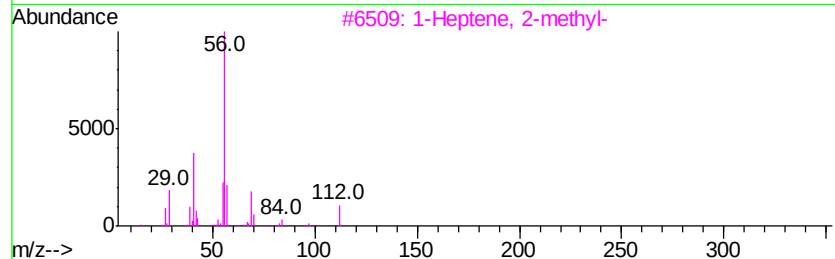
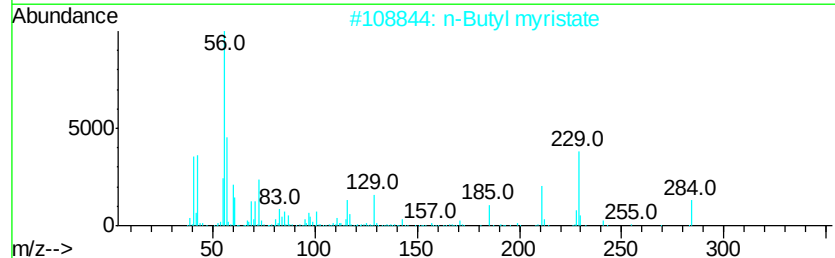
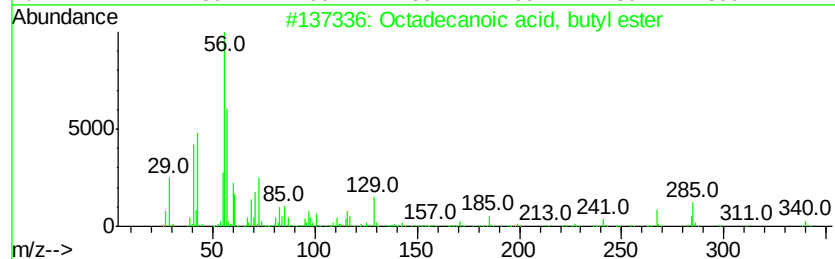
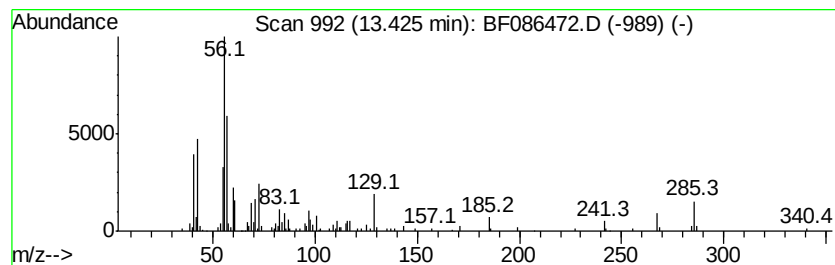
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecanoic acid, butyl ester Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.43	2.99 ng	185534	Chrysene-d12	13.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	91
2		n-Butyl myristate	284	C18H36O2	000110-36-1	72
3		1-Heptene, 2-methyl-	112	C8H16	015870-10-7	38
4		Cyclobutane, ethyl-	84	C6H12	004806-61-5	38
5		Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042816\
Data File : BF086472.D
Acq On : 28 Apr 2016 19:29
Operator : UM/SJ
Sample : H2702-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

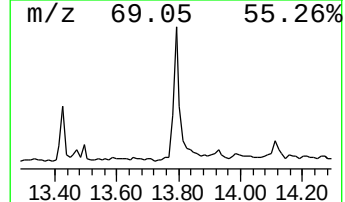
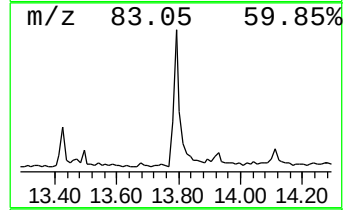
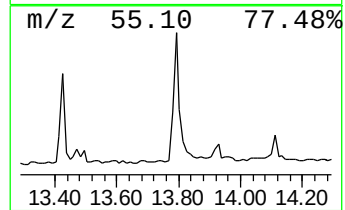
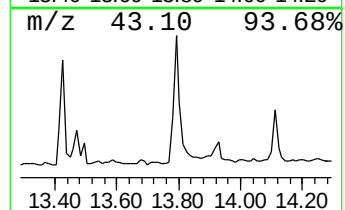
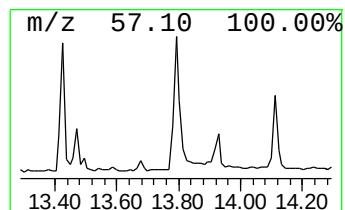
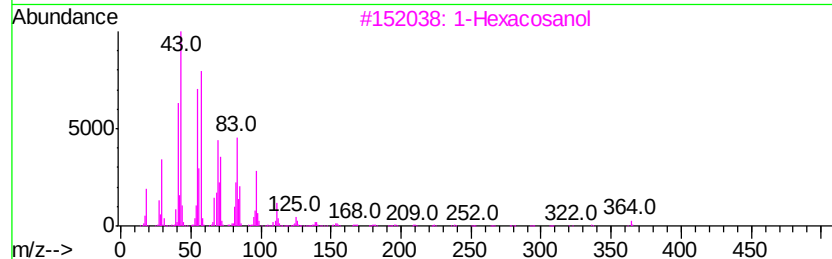
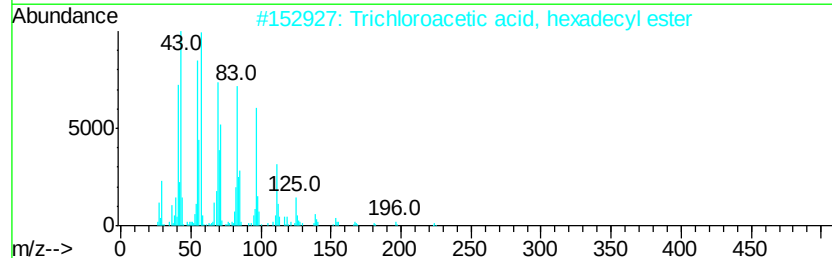
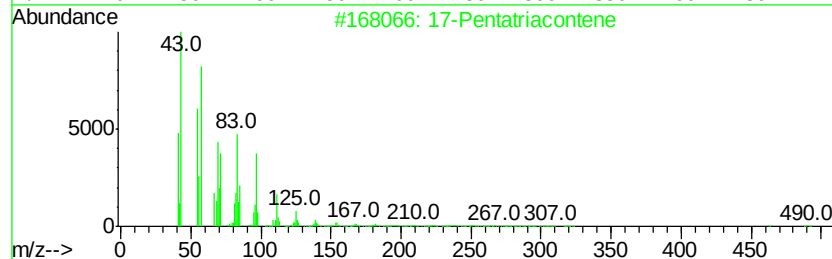
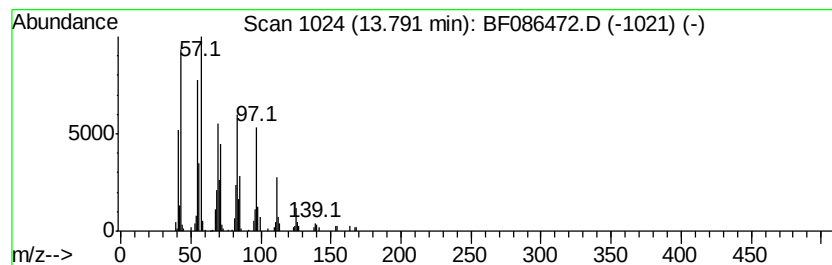
Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 17-Pentatriacontene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	4.36 ng	270095	Chrysene-d12	13.94
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	17-Pentatriacontene	491 C35H70	006971-40-0	91
2	Trichloroacetic acid, hexadecyl ...	386 C18H33Cl3O2	074339-54-1	87
3	1-Hexacosanol	382 C26H54O	000506-52-5	83
4	1-Tetracosanol	354 C24H50O	000506-51-4	80
5	Pentafluoropropionic acid, octad...	416 C21H37F5O2	1000280-07-7	74



Data Path : Z:\HPCHEM1\BNA F\DATA\BF042816\
Data File : BF086472.D
Acq On : 28 Apr 2016 19:29
Operator : UM/SJ
Sample : H2702-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TEC-COMP-B1D

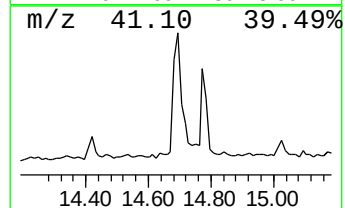
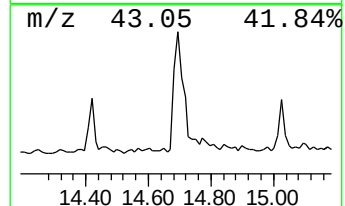
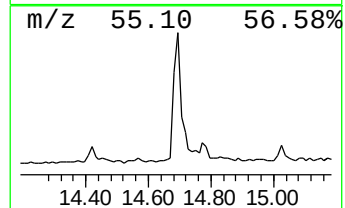
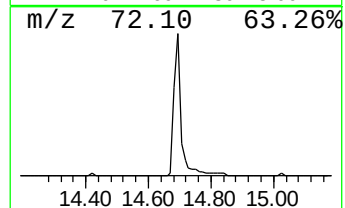
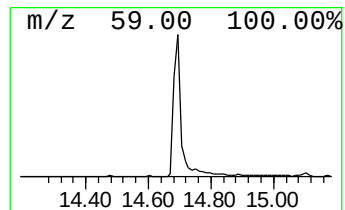
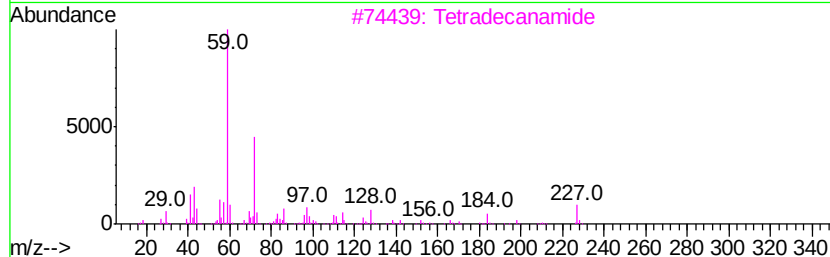
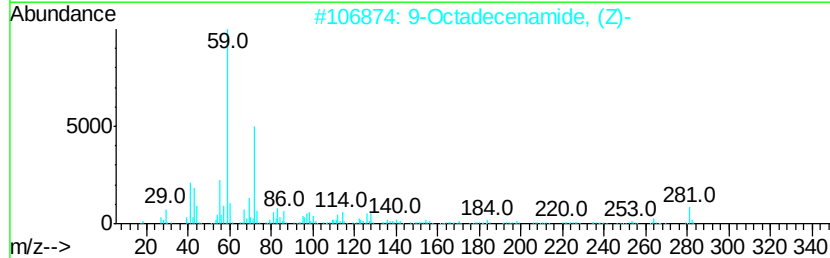
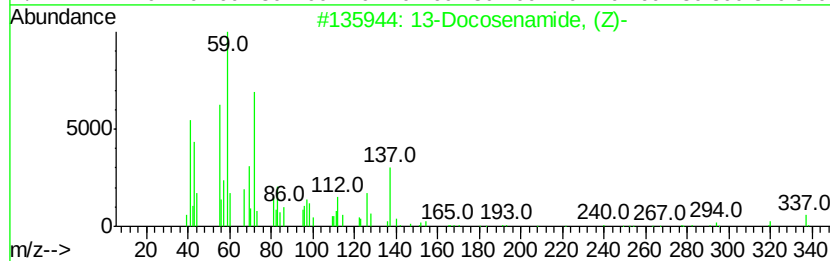
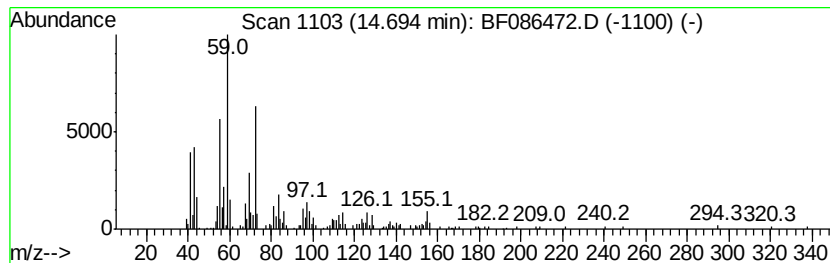
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 13-Docosenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.69	9.92 ng	409152	Perylene-d12	15.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	90
2		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	72
3		Tetradecanamide	227	C14H29NO	000638-58-4	72
4		Hexadecanamide	255	C16H33NO	000629-54-9	64
5		Dodecanamide	199	C12H25NO	001120-16-7	53



Data Path : Z:\HPCHEM1\BNA F\DATA\BF042816\
Data File : BF086472.D
Acq On : 28 Apr 2016 19:29
Operator : UM/SJ
Sample : H2702-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

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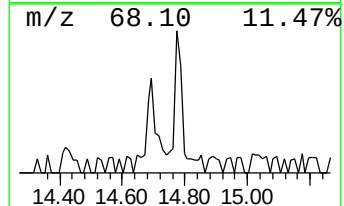
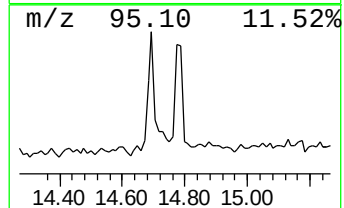
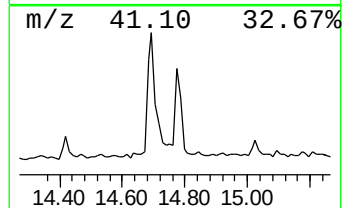
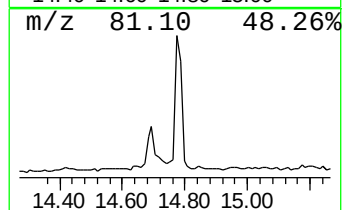
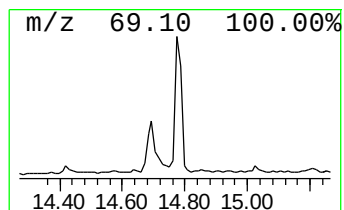
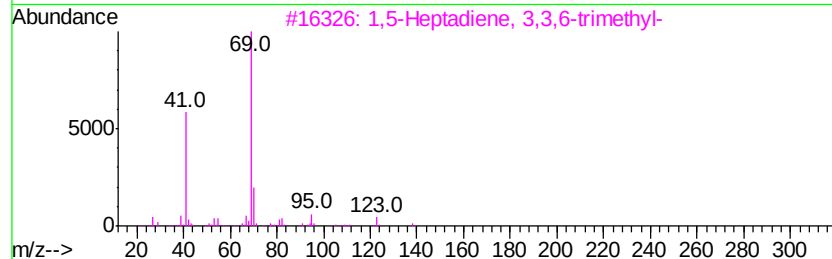
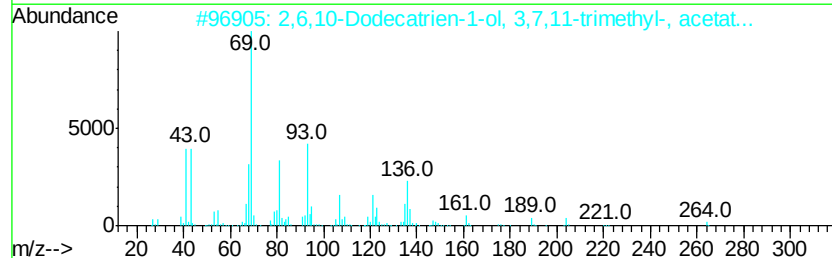
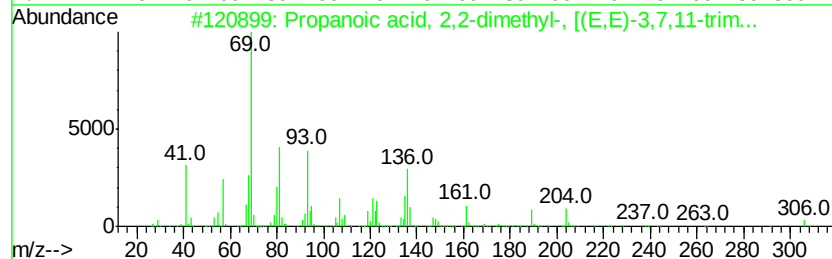
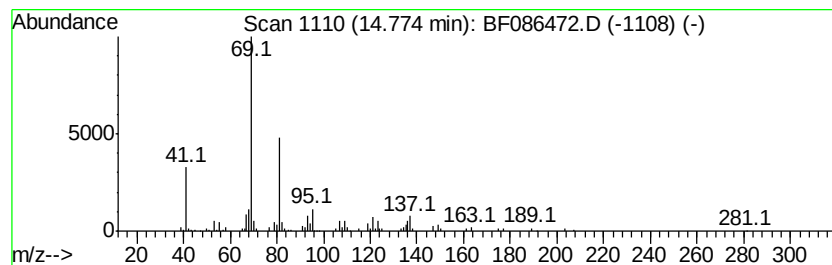
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Propanoic acid, 2,2-dimethy... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.77	3.30 ng	136105	Perylene-d12	15.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanoic acid, 2,2-dimethyl-, [...	306	C20H34O2	1000164-38-8	72
2		2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	72
3		1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	64
4		2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	64
5		2,6-Octadiene, 4-methyl-	124	C9H16	074498-94-5	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042816\
 Data File : BF086472.D
 Acq On : 28 Apr 2016 19:29
 Operator : UM/SJ
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 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.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
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2-Pentanone, 4-hy...	4.97	3.5	ng	172882	1	6.78	1002250	20.0
unknown6.56	6.56	92.4	ng	4632170	1	6.78	1002250	20.0
Hexanoic acid, 2-...	7.45	2.1	ng	130194	2	8.08	1229720	20.0
Hexadecane	10.26	2.2	ng	163188	3	9.82	1499920	20.0
Eicosane	10.74	4.2	ng	283871	4	11.31	1351240	20.0
Hexadecanoic acid...	12.72	4.1	ng	256248	5	13.94	1239910	20.0
Octadecanoic acid...	13.43	3.0	ng	185534	5	13.94	1239910	20.0
17-Pentatriacontene	13.79	4.4	ng	270095	5	13.94	1239910	20.0
13-Docosenamide, ...	14.69	9.9	ng	409152	6	15.33	825029	20.0
Propanoic acid, 2...	14.77	3.3	ng	136105	6	15.33	825029	20.0