

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102615\
 Data File : BF082534.D
 Acq On : 27 Oct 2015 6:33
 Operator : UM/IZ
 Sample : G4116-11
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BT-01(0-2)

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-BF102615.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	4.903	238	242	254	rBV	849868	1660882	55.85%	6.416%
2	5.337	277	280	282	rBV	1886440	2532098	85.14%	9.781%
3	5.726	311	314	318	rVB	31732	35203	1.18%	0.136%
4	6.389	369	372	374	rBV	2083033	2595691	87.28%	10.027%
5	6.503	379	382	384	rBV	2642597	2766043	93.01%	10.685%
6	6.732	400	402	404	rBV	349534	500487	16.83%	1.933%
7	6.880	413	415	418	rBV	2143721	2036449	68.47%	7.867%
8	7.303	449	452	455	rBV	1500045	1576439	53.01%	6.090%
9	8.012	512	514	517	rBV	627824	649928	21.85%	2.511%
10	9.098	606	609	611	rBV	3129580	2974041	100.00%	11.489%
11	9.498	641	644	646	rBV	555694	510040	17.15%	1.970%
12	9.772	665	668	670	rBV	812801	741865	24.94%	2.866%
13	10.195	704	705	707	rVB	30443	33372	1.12%	0.129%
14	10.561	735	737	740	rBV2	1252860	1423942	47.88%	5.501%
15	10.675	745	747	750	rBV	54343	64449	2.17%	0.249%
16	11.121	783	786	787	rBV	50824	44094	1.48%	0.170%
17	11.258	796	798	800	rBV	657587	660084	22.19%	2.550%
18	11.795	843	845	850	rVB	81022	101192	3.40%	0.391%
19	12.469	902	904	907	rBV	85074	78944	2.65%	0.305%
20	12.698	922	924	927	rVB	74129	71901	2.42%	0.278%
21	12.847	934	937	939	rBV	2207126	2112219	71.02%	8.159%
22	13.361	980	982	984	rBV2	35449	42942	1.44%	0.166%
23	13.761	1014	1017	1025	rBV2	90257	202183	6.80%	0.781%
24	13.909	1027	1030	1032	rBV	556817	644789	21.68%	2.491%
25	14.070	1042	1044	1050	rBV6	13221	48253	1.62%	0.186%
26	14.390	1069	1072	1073	rBV2	39578	56905	1.91%	0.220%
27	14.424	1073	1075	1080	rVB3	53226	130270	4.38%	0.503%
28	14.778	1104	1106	1108	rVB	25154	34621	1.16%	0.134%
29	14.847	1110	1112	1115	rVV	42838	56249	1.89%	0.217%
30	14.961	1120	1122	1125	rVV	45939	87154	2.93%	0.337%
31	15.018	1125	1127	1129	rVB	46401	55380	1.86%	0.214%
32	15.064	1129	1131	1136	rBV2	67314	154366	5.19%	0.596%
33	15.247	1145	1147	1149	rBV	23168	35003	1.18%	0.135%
34	15.304	1150	1152	1154	rVV	31310	41471	1.39%	0.160%

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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

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35	15.361	1154	1157	1162	rVV	397063	554155	18.63%	2.141%
36	15.773	1190	1193	1195	rBV	36174	68026	2.29%	0.263%
37	16.721	1272	1276	1277	rBV4	34287	82917	2.79%	0.320%
38	16.813	1281	1284	1287	rVV2	60996	104686	3.52%	0.404%
39	17.236	1317	1321	1328	rVB6	36871	145687	4.90%	0.563%
40	17.876	1375	1377	1381	rVB3	28144	67166	2.26%	0.259%
41	18.138	1396	1400	1405	rVB3	34604	105421	3.54%	0.407%

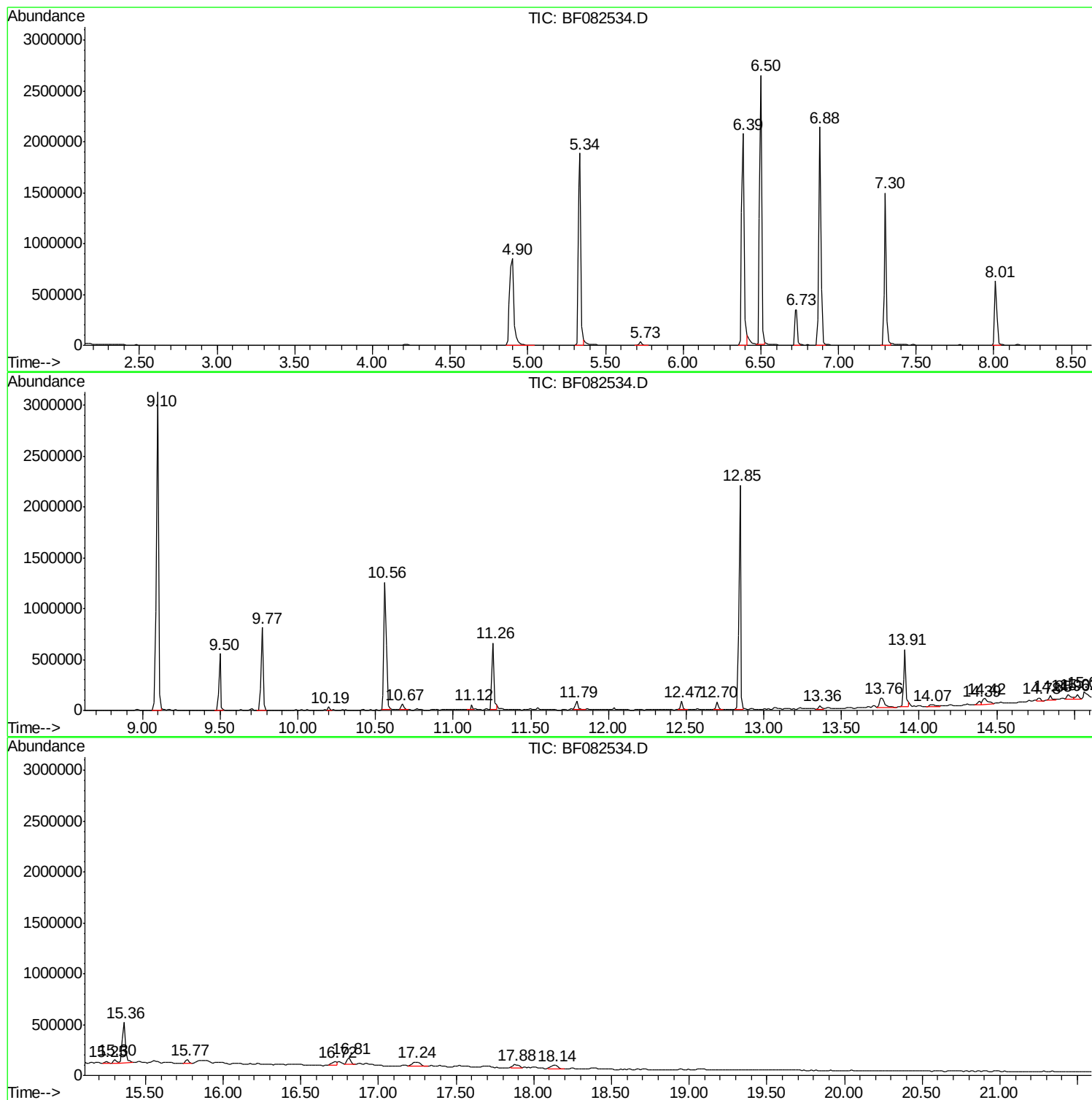
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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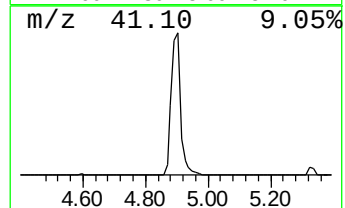
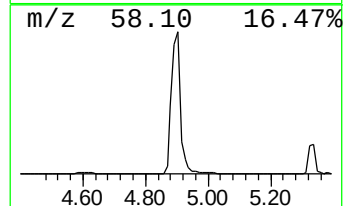
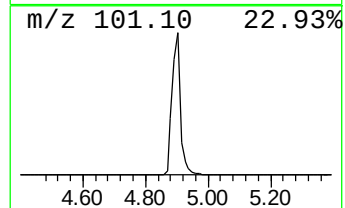
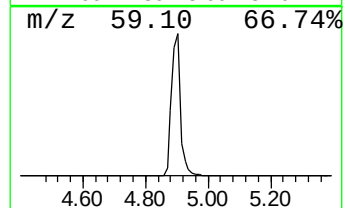
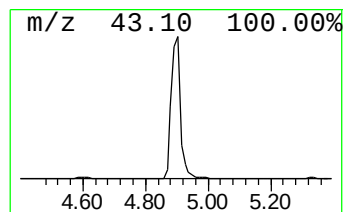
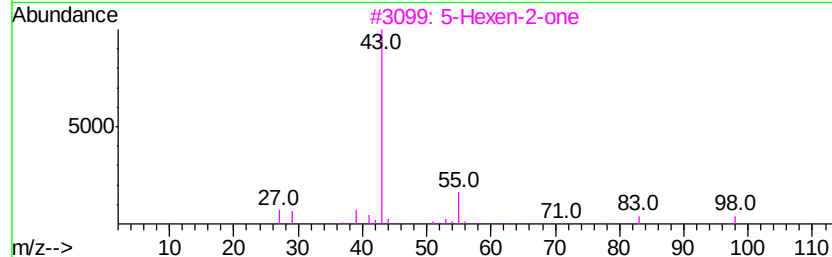
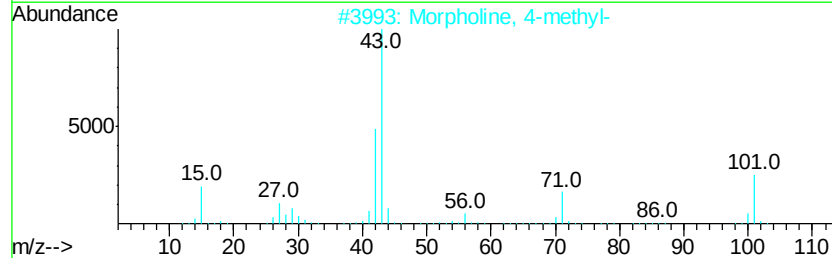
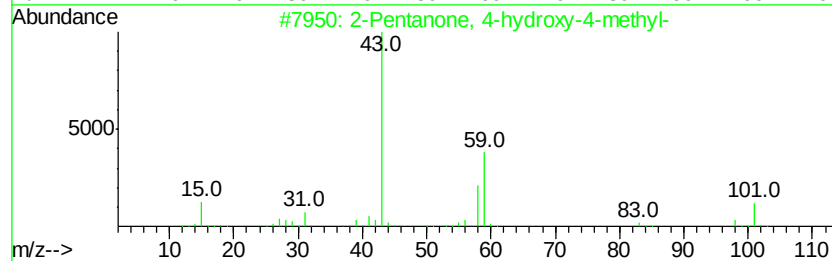
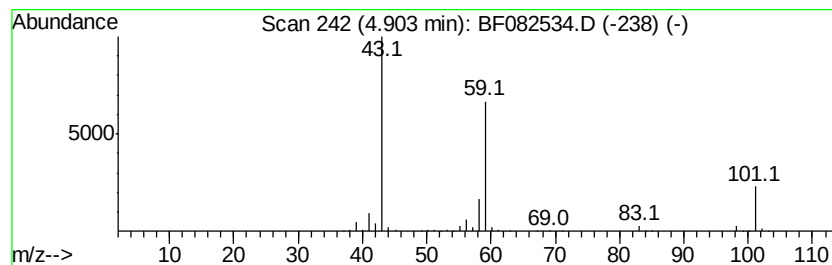
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.90	66.37 ng	1660880	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
3		5-Hexen-2-one	98	C6H10O	000109-49-9	9
4		Guanidine	59	CH5N3	000113-00-8	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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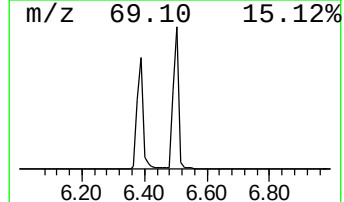
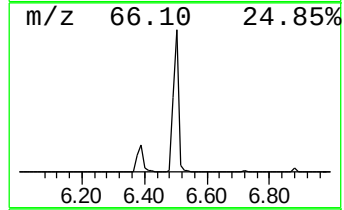
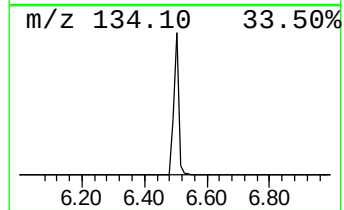
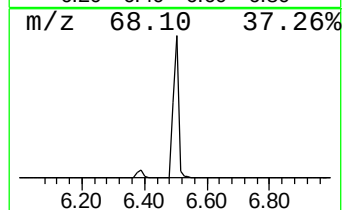
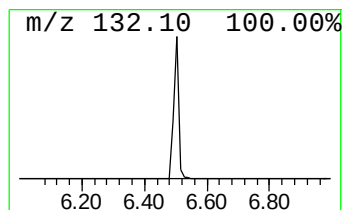
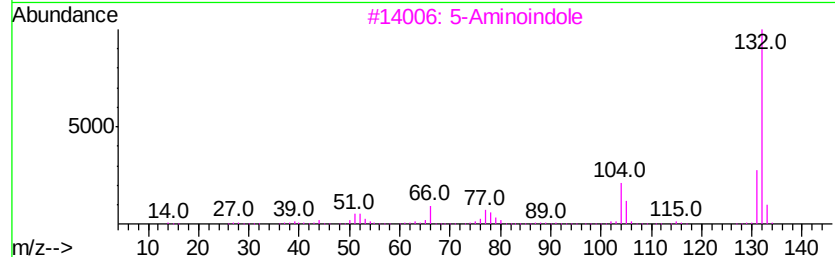
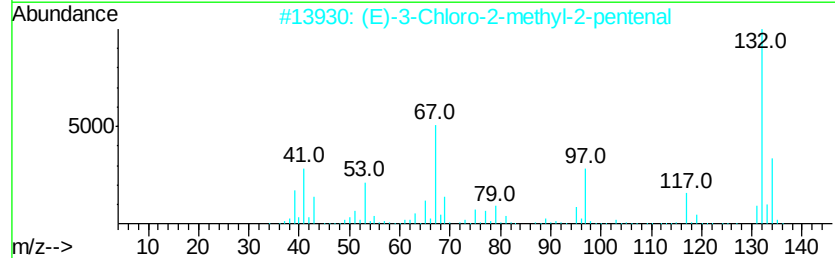
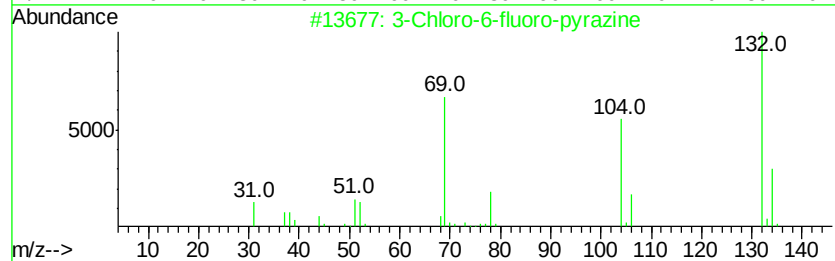
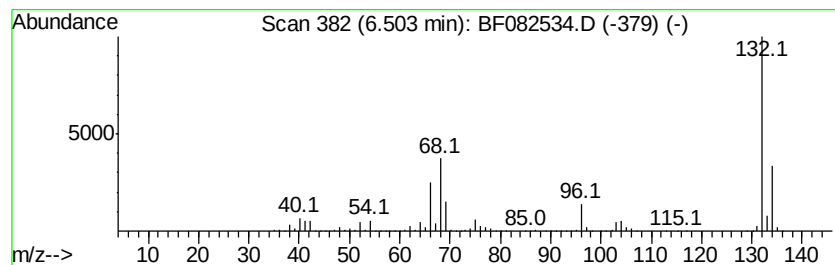
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Peak Number 2 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	110.53 ng	2766040	1,4-Dichlorobenzene-d4	6.73

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		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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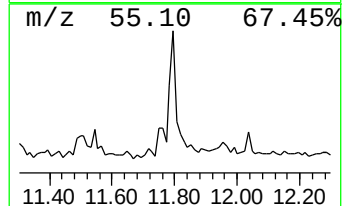
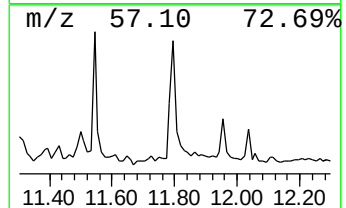
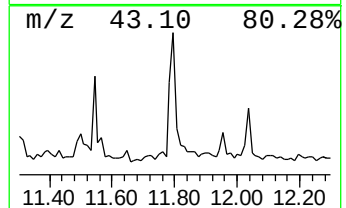
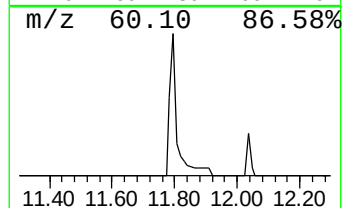
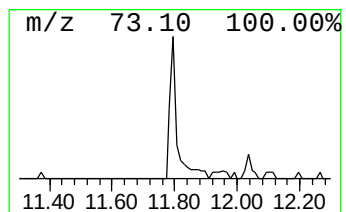
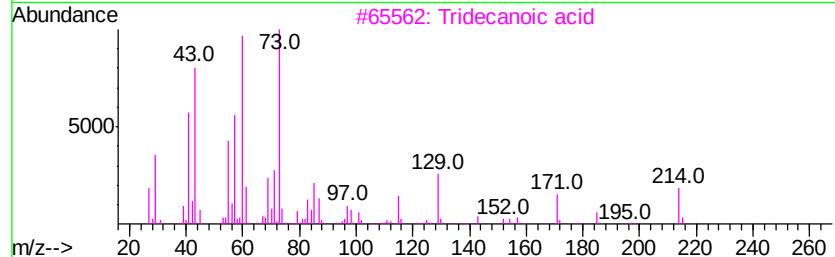
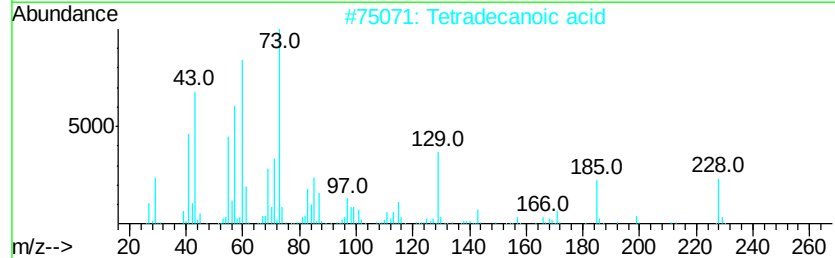
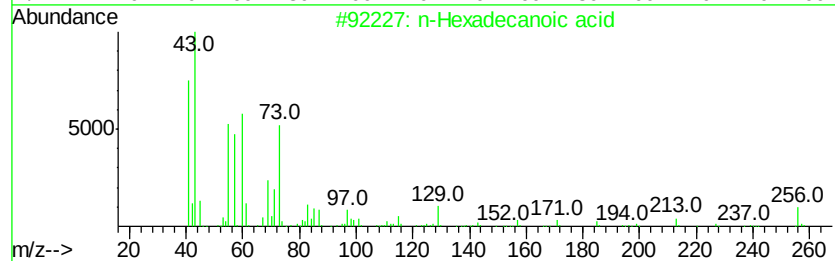
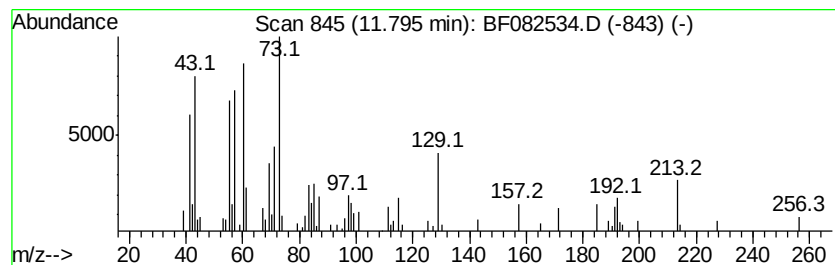
Instrument :
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ClientSampleId :
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.80	3.07 ng	101192	Phenanthrene-d10	11.26	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
3	Tridecanoic acid	214	C13H26O2	000638-53-9	76
4	Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	11
5	Dodecane	170	C12H26	000112-40-3	11



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Instrument :
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ClientSampled :
BT-01(0-2)

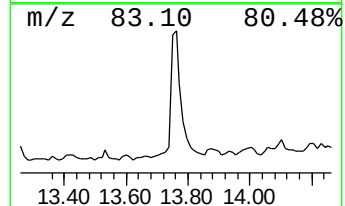
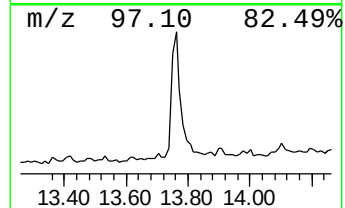
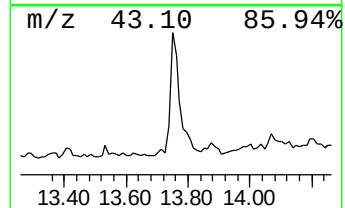
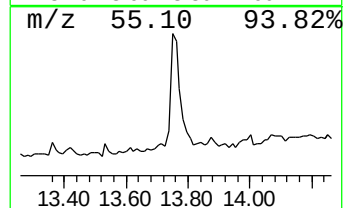
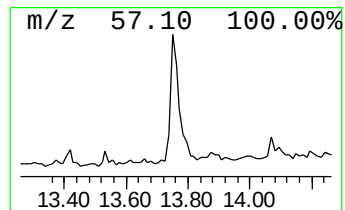
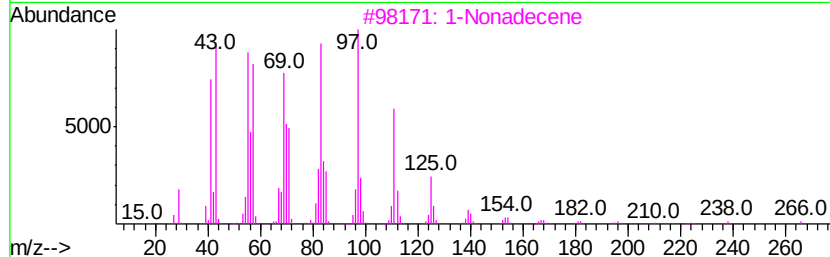
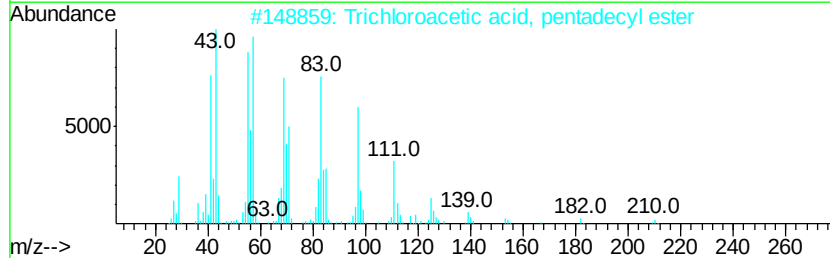
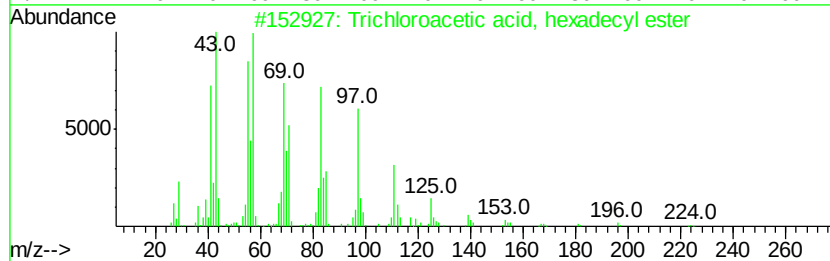
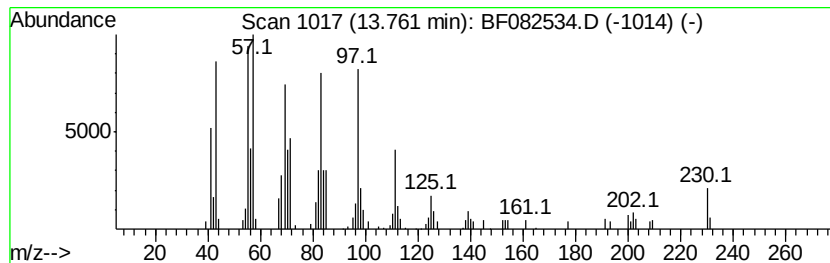
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Trichloroacetic acid, hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.76	6.27 ng	202183	Chrysene-d12	13.91

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
2		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
3		1-Nonadecene	266	C19H38	018435-45-5	91
4		11-Tricosene	322	C23H46	052078-56-5	91
5		3-Eicosene, (E)-	280	C20H40	074685-33-9	91



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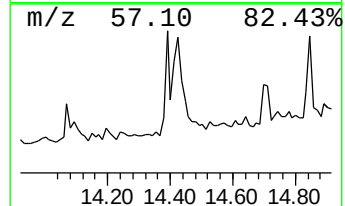
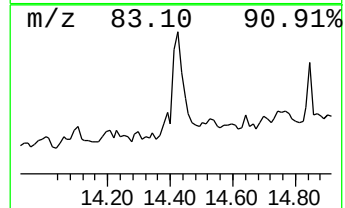
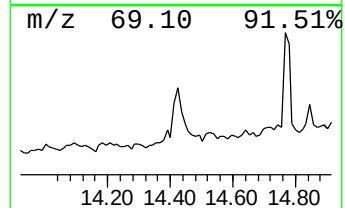
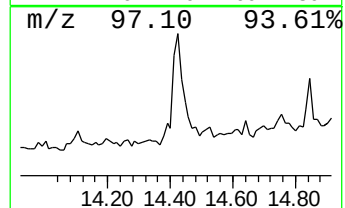
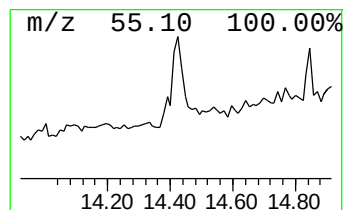
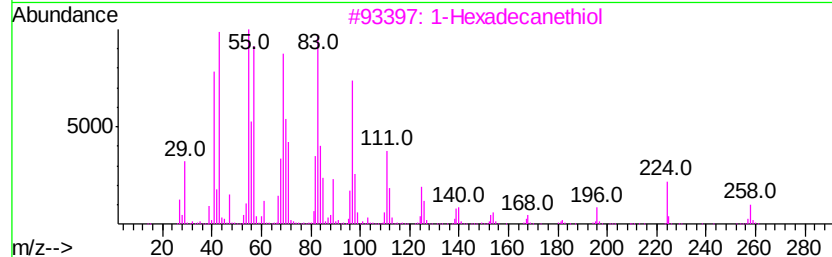
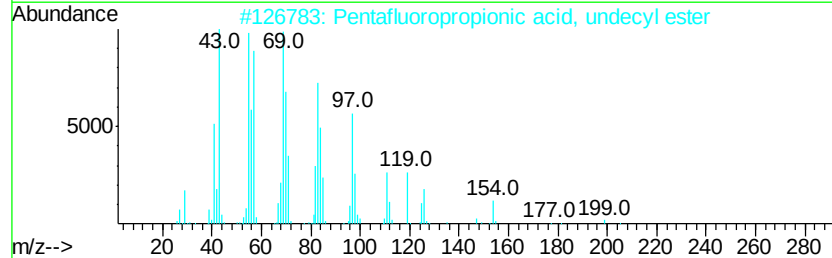
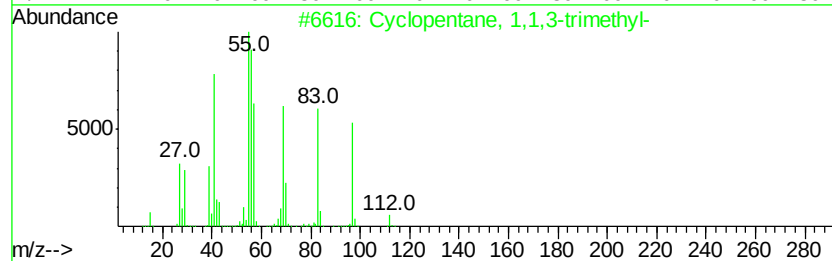
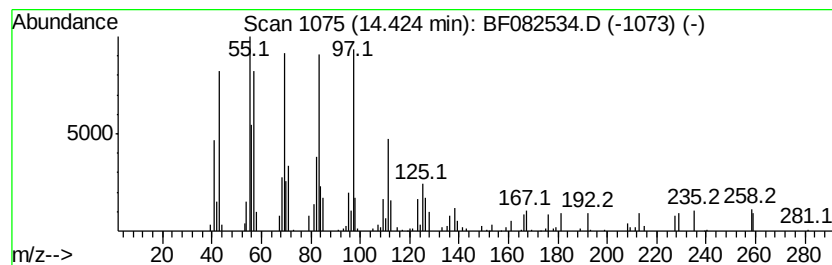
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Cyclopentane, 1,1,3-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.42	4.04 ng	130270	Chrysene-d12	13.91

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	52
2		Pentafluoropropionic acid, undec...	318	C14H23F5O2	1000283-04-0	49
3		1-Hexadecanethiol	258	C16H34S	002917-26-2	49
4		Cyclohexane, 1,2,4-trimethyl-	126	C9H18	002234-75-5	41
5		Isoheptadecanol	256	C17H36O	057289-07-3	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102615\
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Acq On : 27 Oct 2015 6:33
Operator : UM/IZ
Sample : G4116-11
Misc :
ALS Vial : 17 Sample Multiplier: 1

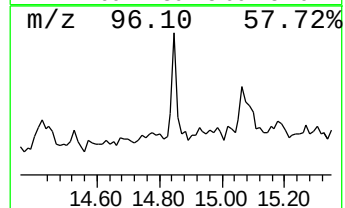
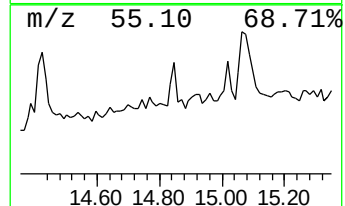
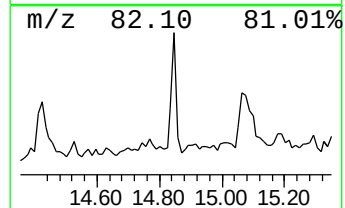
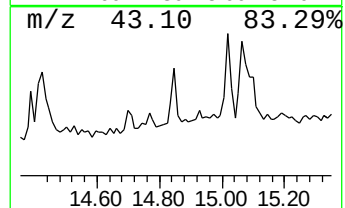
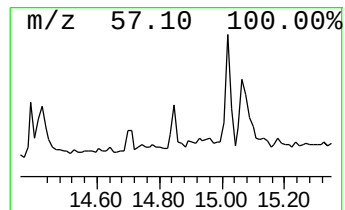
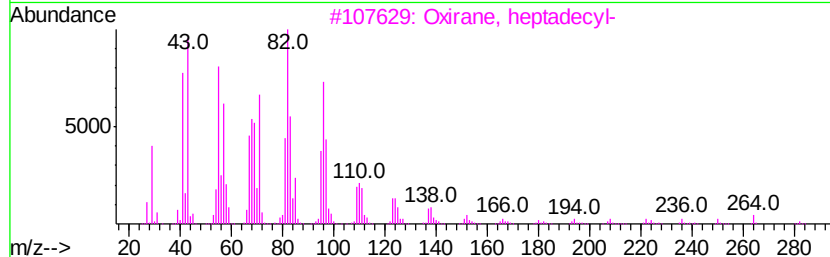
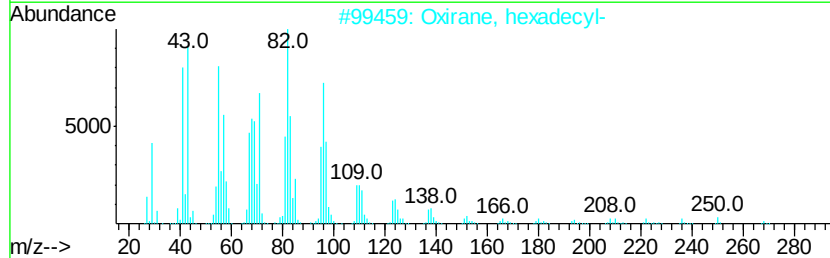
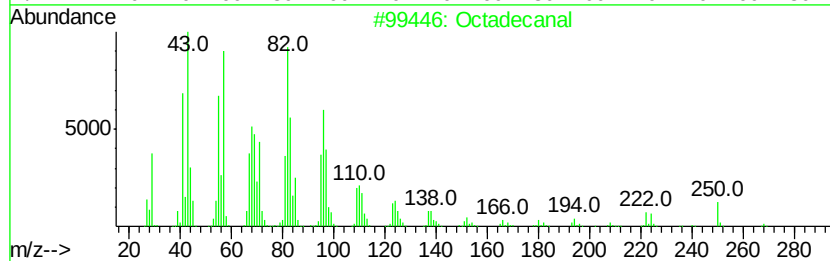
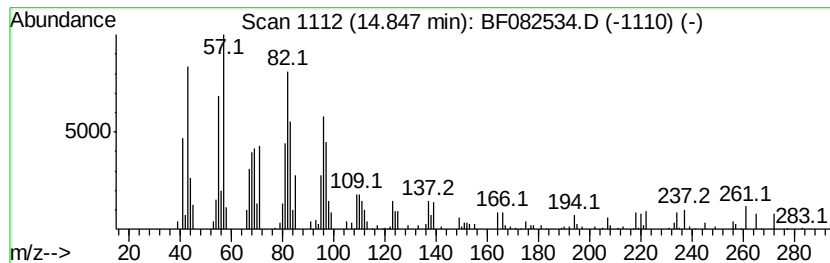
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanal Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.85	2.03 ng	56249	Perylene-d12	15.36	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	81
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	74
3	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	68
4	17-Octadecenal	266	C18H34O	056554-86-0	64
5	1,19-Eicosadiene	278	C20H38	014811-95-1	62



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102615\
Data File : BF082534.D
Acq On : 27 Oct 2015 6:33
Operator : UM/IZ
Sample : G4116-11
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
BT-01(0-2)

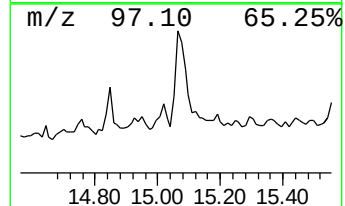
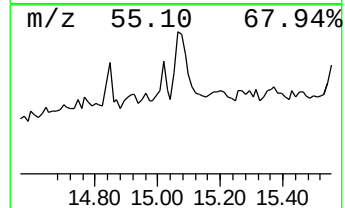
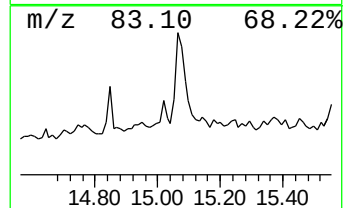
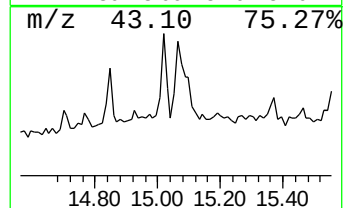
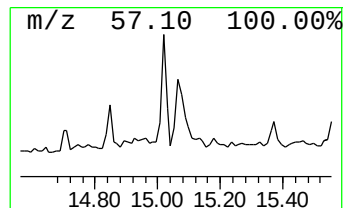
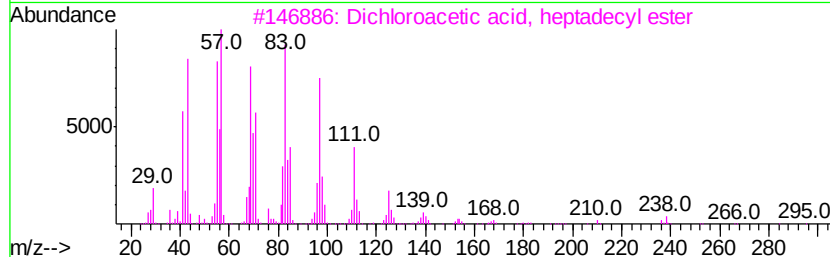
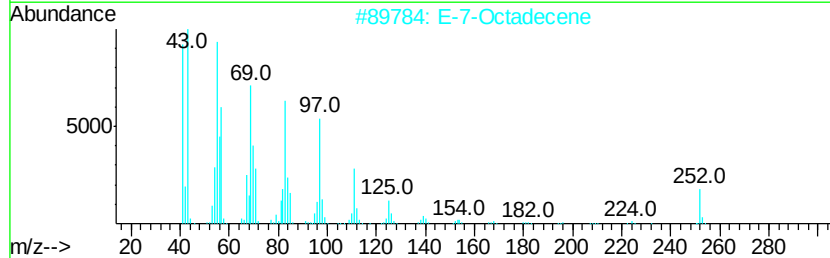
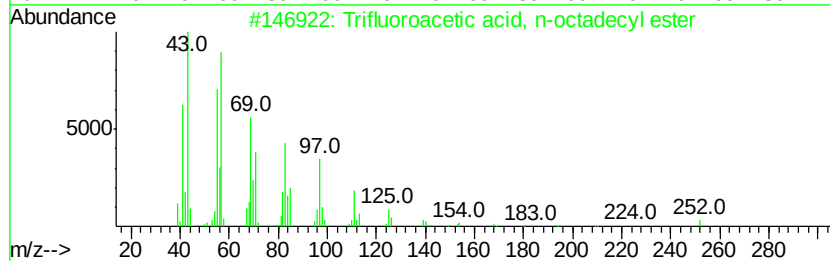
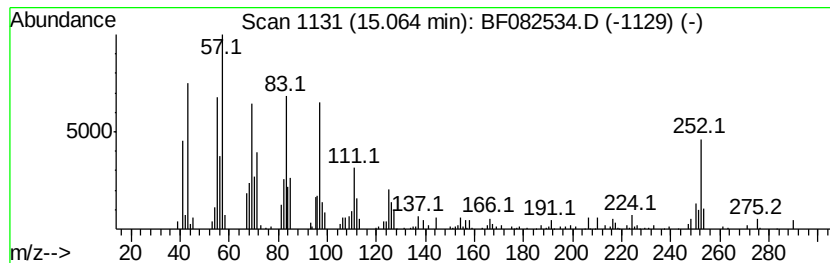
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Trifluoroacetic acid, n-oct... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.06	5.57 ng	154366	Perylene-d12	15.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trifluoroacetic acid, n-octadecyl...	366	C20H37F3O2	079392-43-1	81
2		E-7-Octadecene	252	C18H36	1000130-92-0	81
3		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	70
4		Cyclohexadecane	224	C16H32	000295-65-8	70
5		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	70



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102615\
Data File : BF082534.D
Acq On : 27 Oct 2015 6:33
Operator : UM/IZ
Sample : G4116-11
Misc :
ALS Vial : 17 Sample Multiplier: 1

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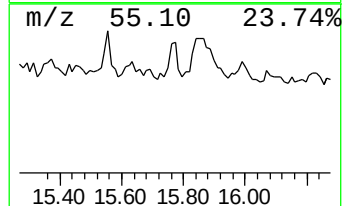
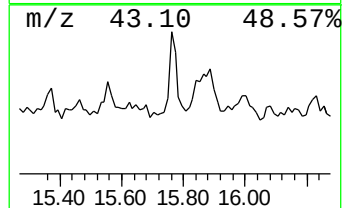
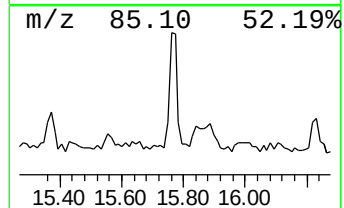
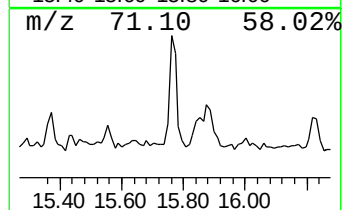
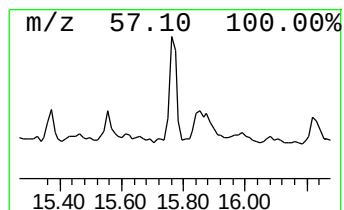
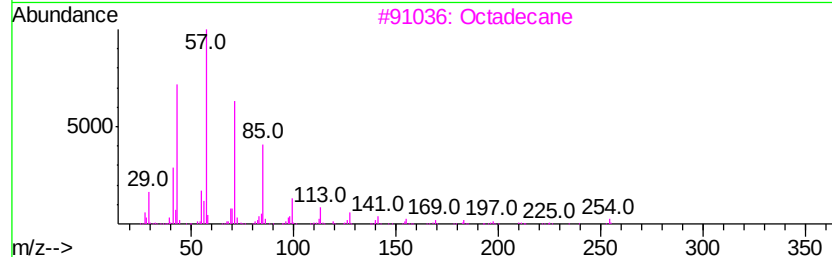
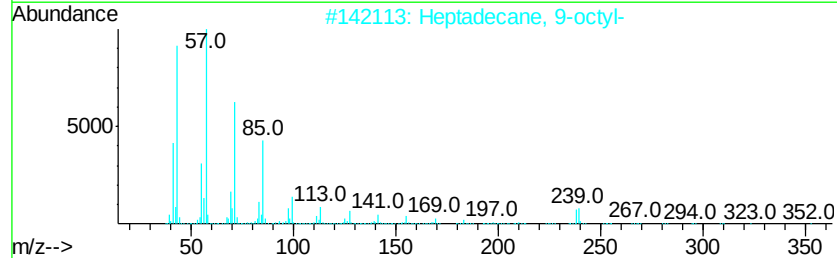
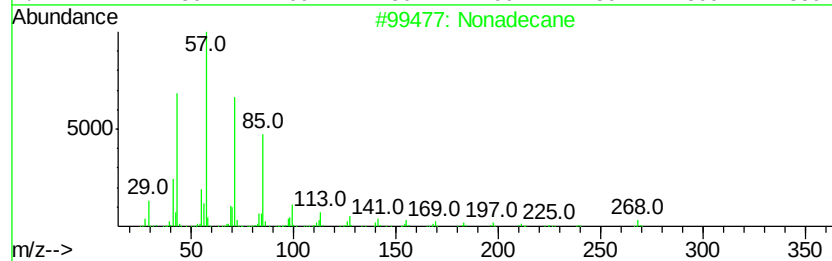
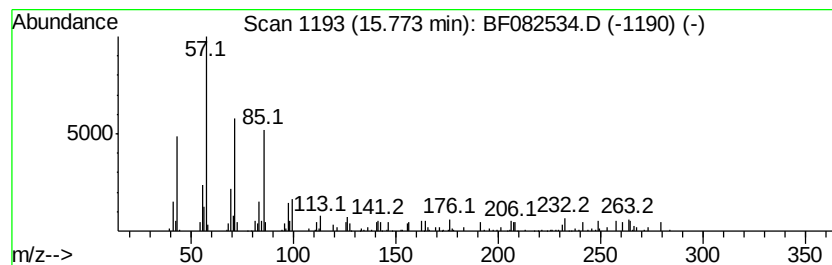
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Nonadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.77	2.46 ng	68026	Perylene-d12	15.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecane	268	C19H40	000629-92-5	52
2		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	52
3		Octadecane	254	C18H38	000593-45-3	52
4		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	50
5		Eicosane, 10-methyl-	296	C21H44	054833-23-7	50



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102615\
Data File : BF082534.D
Acq On : 27 Oct 2015 6:33
Operator : UM/IZ
Sample : G4116-11
Misc :
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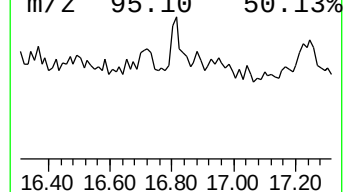
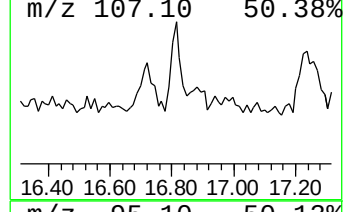
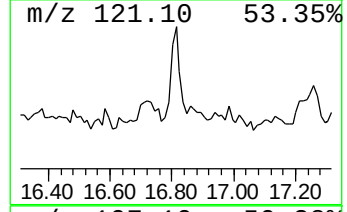
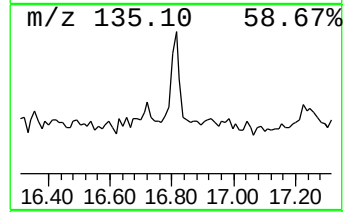
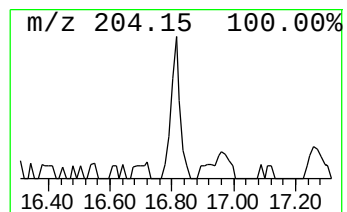
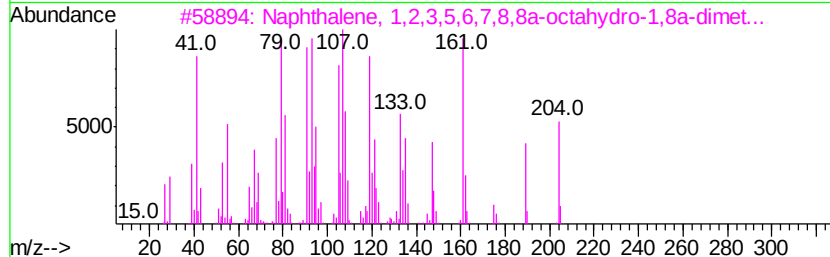
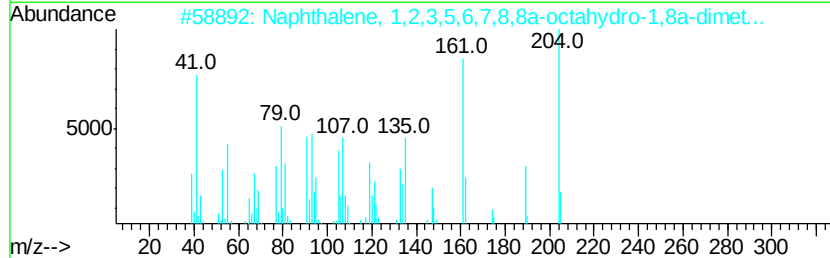
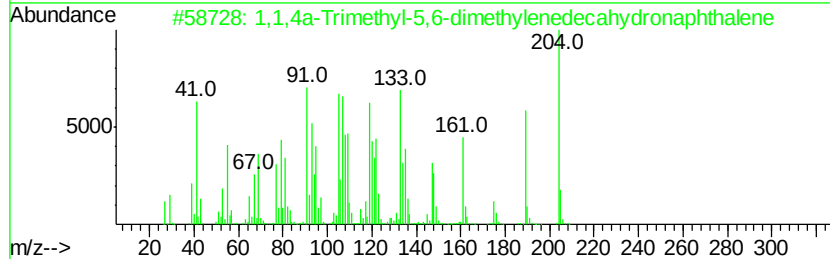
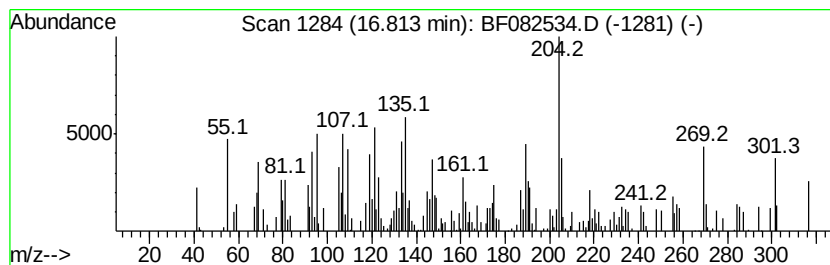
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 1,1,4a-Trimethyl-5,6-dimeth... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.81	3.78 ng	104686	Perylene-d12	15.36	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	89
2	Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	78
3	Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	010219-75-7	53
4	1,2,4,8-Tetramethylbicyclo[6.3.0]...	204	C15H24	137235-51-9	46
5	1H-3a,7-Methanoazulene, 2,3,6,7,...	204	C15H24	000560-32-7	45



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102615\
Data File : BF082534.D
Acq On : 27 Oct 2015 6:33
Operator : UM/IZ
Sample : G4116-11
Misc :
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Instrument :
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ClientSampleId :
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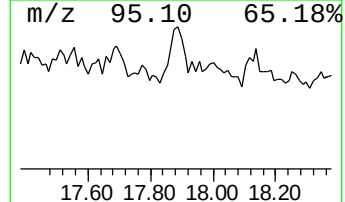
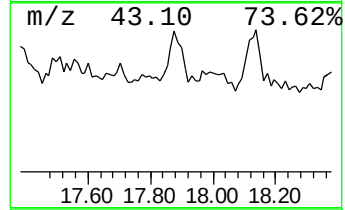
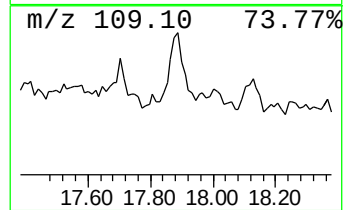
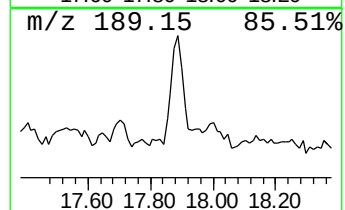
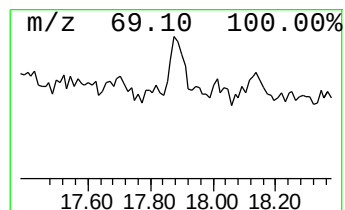
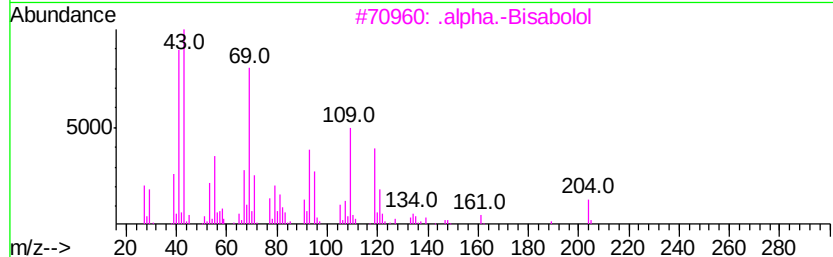
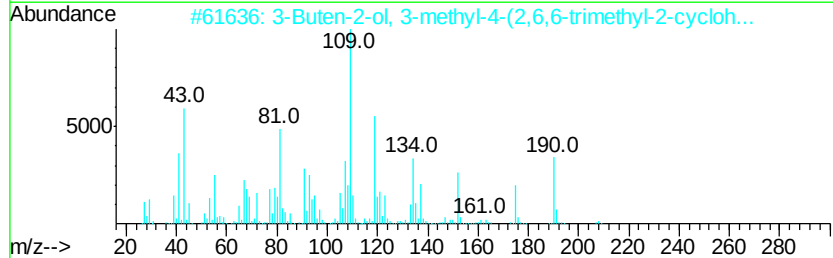
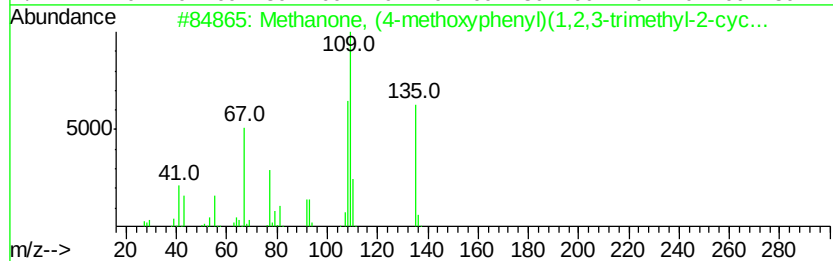
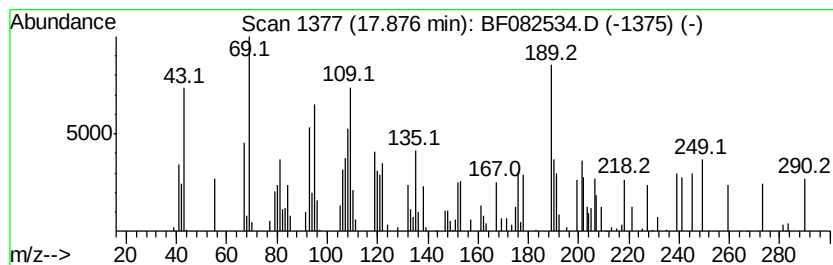
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown17.88 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.88	2.42 ng	67166	Perylene-d12	15.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methanone, (4-methoxyphenyl)(1,2...	244	C16H20O2	1000197-56-3	27
2		3-Buten-2-ol, 3-methyl-4-(2,6,6-...	208	C14H24O	070172-00-8	22
3		.alpha.-Bisabolol	222	C15H26O	000515-69-5	14
4		Butanoic acid, 2-methyl-4-nitro-...	251	C13H17NO4	1000196-62-4	14
5		1,10-Dimethyl-2-methylene-trans-...	178	C13H22	1000103-97-8	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102615\
Data File : BF082534.D
Acq On : 27 Oct 2015 6:33
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Misc :
ALS Vial : 17 Sample Multiplier: 1

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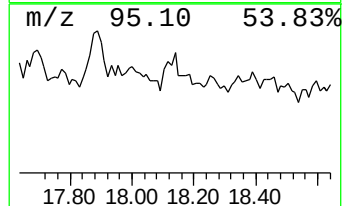
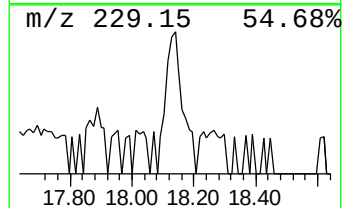
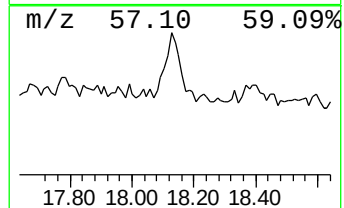
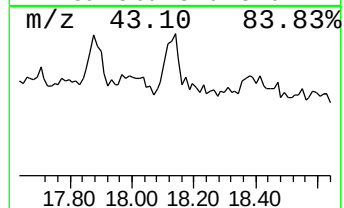
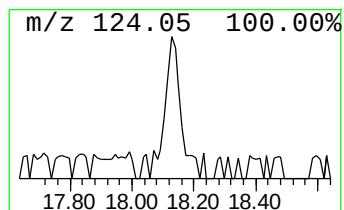
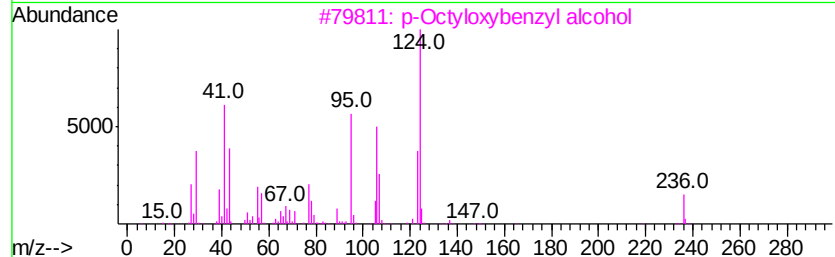
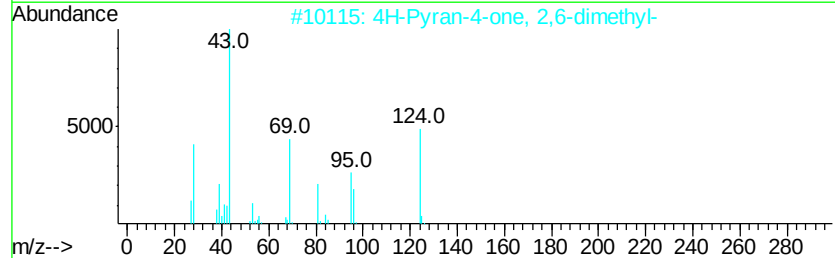
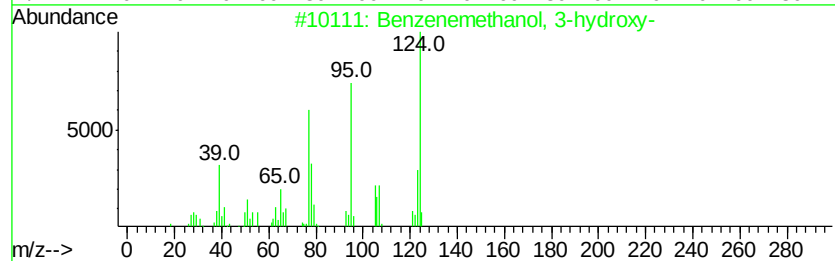
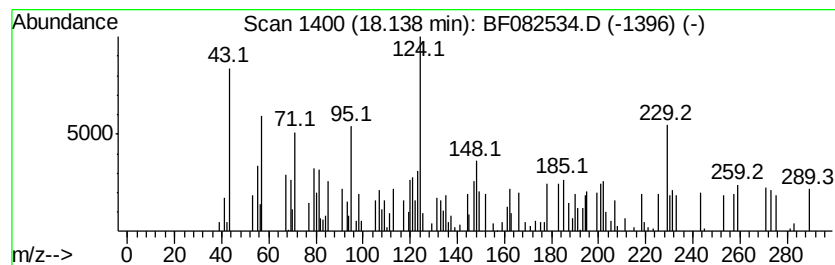
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 unknown18.14 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.14	3.80 ng	105421	Perylene-d12	15.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzenemethanol, 3-hydroxy-	124	C7H8O2	000620-24-6	30
2		4H-Pyran-4-one, 2,6-dimethyl-	124	C7H8O2	001004-36-0	27
3		p-Octyloxybenzyl alcohol	236	C15H24O2	067698-68-4	27
4		3-Methyl-2-pyrazinylmethanol	124	C6H8N2O	160818-32-6	27
5		1,3-Benzenediol, 5-pentyl-	180	C11H16O2	000500-66-3	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102615\
 Data File : BF082534.D
 Acq On : 27 Oct 2015 6:33
 Operator : UM/IZ
 Sample : G4116-11
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
 BT-01(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102615.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...	4.90	66.4	ng	1660880	1	6.73	500487	20.0
unknown6.50	6.50	110.5	ng	2766040	1	6.73	500487	20.0
n-Hexadecanoic acid	11.80	3.1	ng	101192	4	11.26	660084	20.0
Trichloroacetic a...	13.76	6.3	ng	202183	5	13.91	644789	20.0
Cyclopentane, 1,1...	14.42	4.0	ng	130270	5	13.91	644789	20.0
Octadecanal	14.85	2.0	ng	56249	6	15.36	554155	20.0
Trifluoroacetic a...	15.06	5.6	ng	154366	6	15.36	554155	20.0
Nonadecane	15.77	2.5	ng	68026	6	15.36	554155	20.0
1,1,4a-Trimethyl-...	16.81	3.8	ng	104686	6	15.36	554155	20.0
unknown17.88	17.88	2.4	ng	67166	6	15.36	554155	20.0
unknown18.14	18.14	3.8	ng	105421	6	15.36	554155	20.0