

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102115\
 Data File : BF082430.D
 Acq On : 22 Oct 2015 4:37
 Operator : UM/IZ
 Sample : G4116-11
 Misc :
 ALS Vial : 29 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-BF101015.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	4.937	242	245	257	rBV	821523	1456409	56.42%	6.407%
2	5.371	280	283	285	rBV	2208907	2327271	90.16%	10.238%
3	5.771	316	318	320	rVB	23294	26762	1.04%	0.118%
4	6.423	372	375	377	rBV	1852928	2334548	90.44%	10.270%
5	6.537	383	385	388	rBV	2217537	2176165	84.30%	9.573%
6	6.766	403	405	408	rBV	473659	461409	17.87%	2.030%
7	6.926	416	419	421	rBV	2182320	1947456	75.44%	8.567%
8	7.349	453	456	458	rBV	973461	1410529	54.64%	6.205%
9	8.057	516	518	520	rBV	733058	602024	23.32%	2.648%
10	9.143	610	613	615	rBV	2360018	2581339	100.00%	11.356%
11	9.532	645	647	650	rBV	373840	393126	15.23%	1.729%
12	9.818	669	672	674	rBV	528054	586963	22.74%	2.582%
13	10.240	708	709	711	rVB	34202	29866	1.16%	0.131%
14	10.606	738	741	743	rBV	1263199	1203865	46.64%	5.296%
15	10.720	749	751	754	rBV	44286	57088	2.21%	0.251%
16	11.166	788	790	791	rBV	44370	37865	1.47%	0.167%
17	11.303	800	802	804	rBV	427100	498752	19.32%	2.194%
18	11.829	847	848	851	rBV2	86535	107537	4.17%	0.473%
19	12.515	905	908	910	rBV	61866	65297	2.53%	0.287%
20	12.744	924	928	930	rBV	58870	66603	2.58%	0.293%
21	12.892	938	941	943	rBV	1842314	1747000	67.68%	7.685%
22	13.406	984	986	989	rBV	27526	34973	1.35%	0.154%
23	13.589	999	1002	1004	rBV	22245	29874	1.16%	0.131%
24	13.795	1019	1020	1027	rVB2	99402	181846	7.04%	0.800%
25	13.955	1031	1034	1039	rVV	547905	595235	23.06%	2.619%
26	14.127	1047	1049	1054	rBV4	14277	37165	1.44%	0.163%
27	14.469	1075	1079	1087	rBV4	59670	228518	8.85%	1.005%
28	14.847	1110	1112	1113	rBV	33593	38798	1.50%	0.171%
29	14.915	1116	1118	1121	rVV	54784	62765	2.43%	0.276%
30	15.018	1125	1127	1131	rVV	41830	82404	3.19%	0.363%
31	15.098	1131	1134	1135	rVV	40549	57490	2.23%	0.253%
32	15.132	1135	1137	1144	rVV4	50861	135939	5.27%	0.598%
33	15.429	1160	1163	1169	rBV	397974	582936	22.58%	2.564%
34	15.864	1199	1201	1203	rBV	41181	61074	2.37%	0.269%

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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-BF101015.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.812	1282	1284	1288	rVB3	35560	83964	3.25%	0.369%
36	16.938	1292	1295	1301	rBV4	60364	140514	5.44%	0.618%
37	17.350	1327	1331	1333	rBV4	35288	95233	3.69%	0.419%
38	18.047	1390	1392	1397	rVB5	30868	63098	2.44%	0.278%
39	18.287	1410	1413	1420	rVB5	33639	101798	3.94%	0.448%

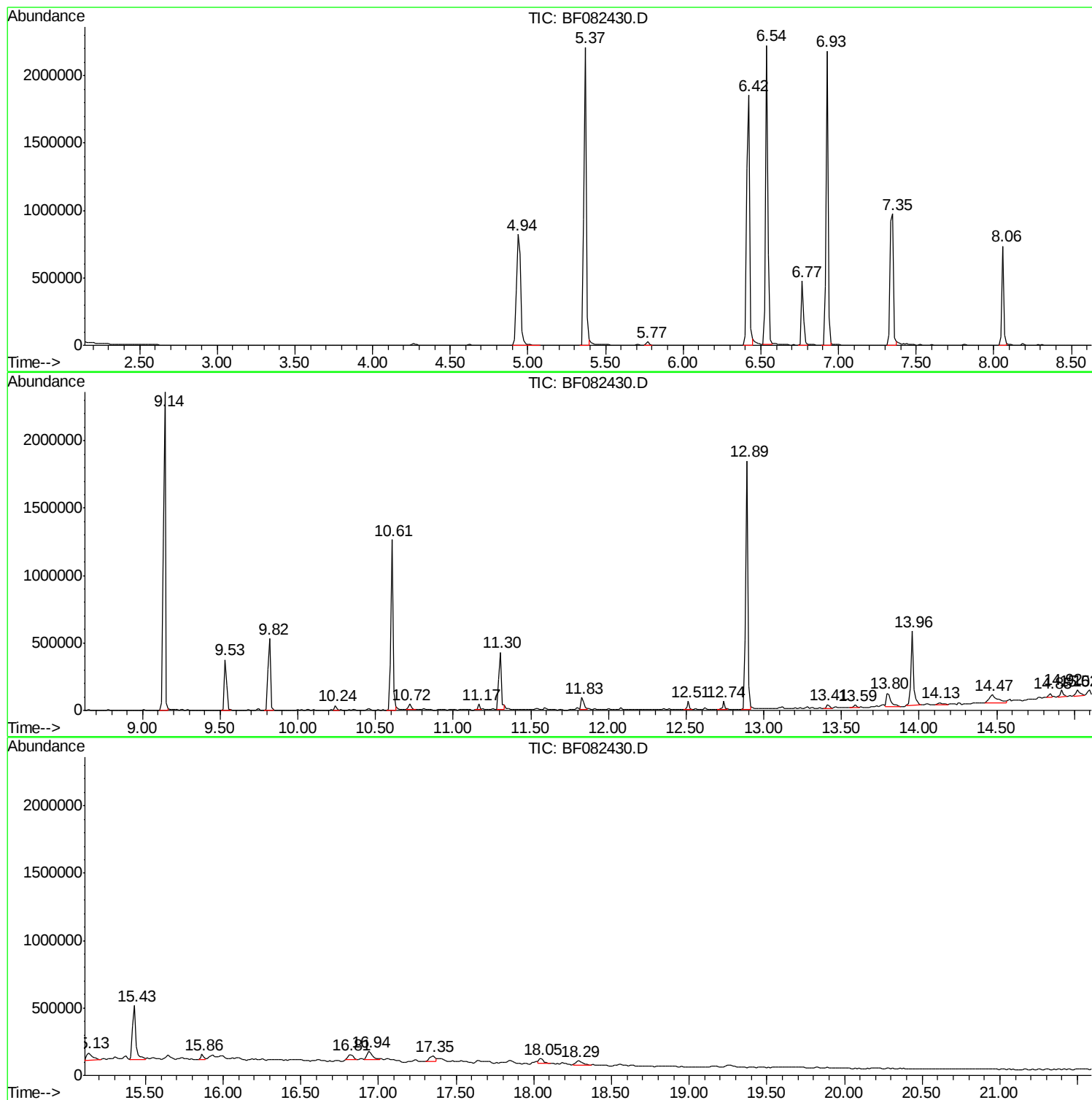
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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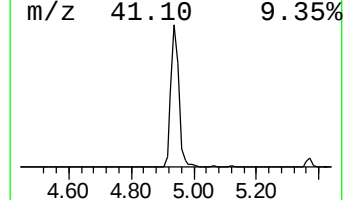
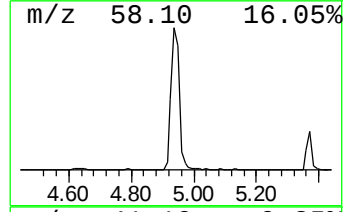
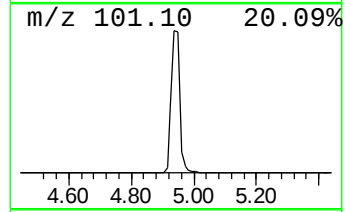
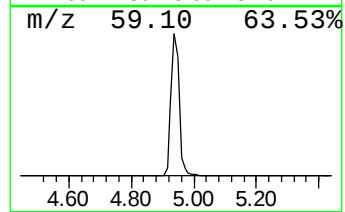
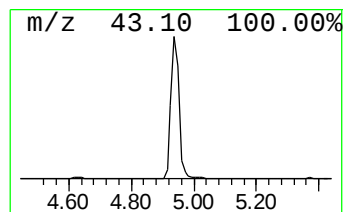
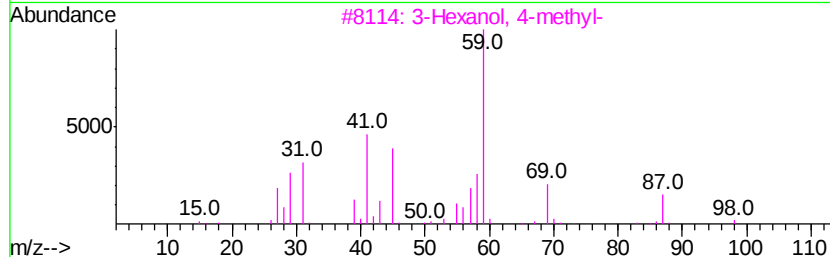
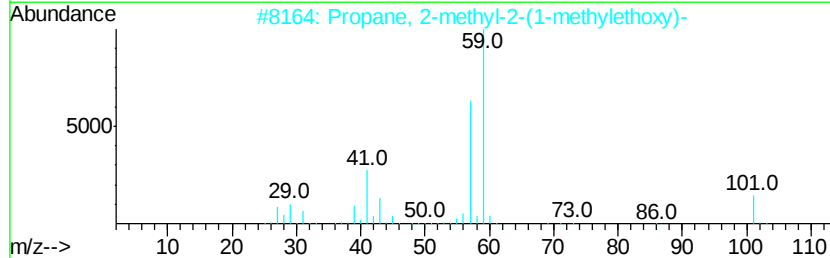
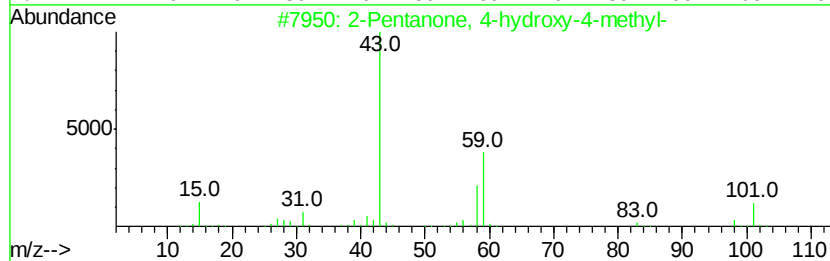
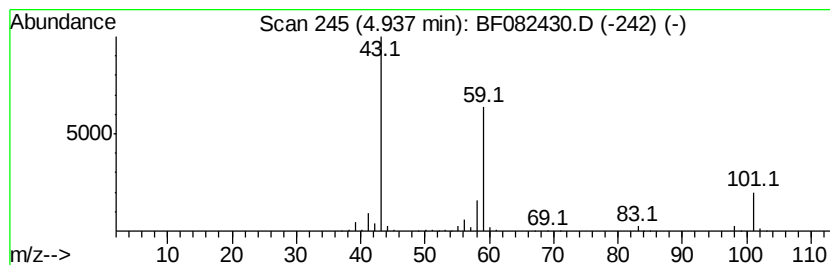
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.94	63.13 ng	1456410	1,4-Dichlorobenzene-d4	6.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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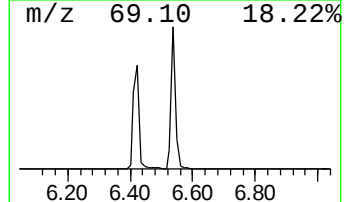
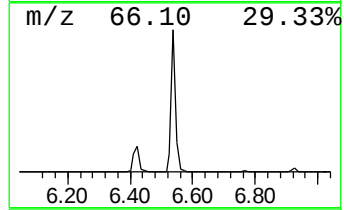
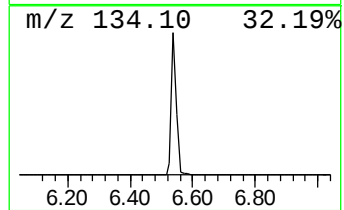
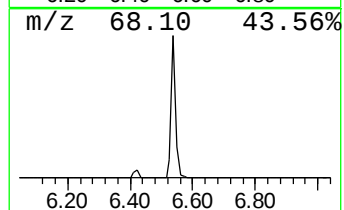
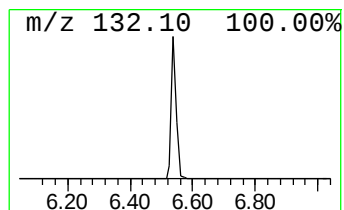
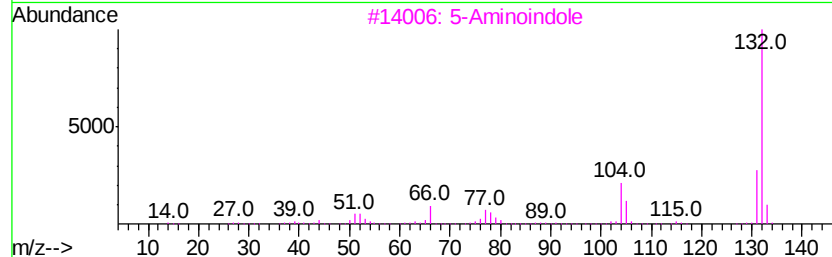
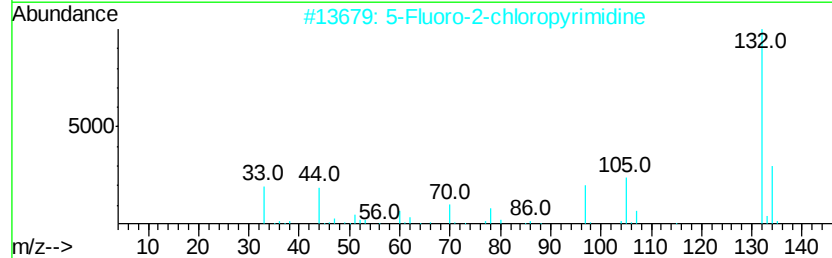
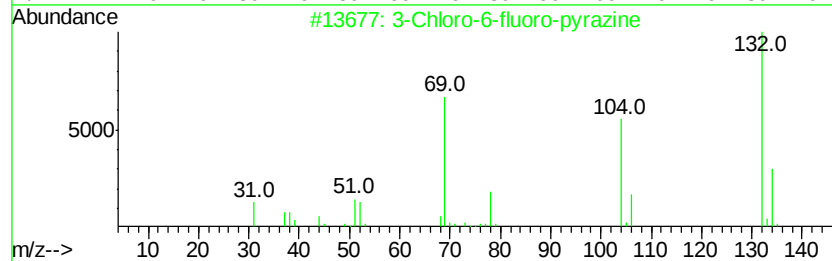
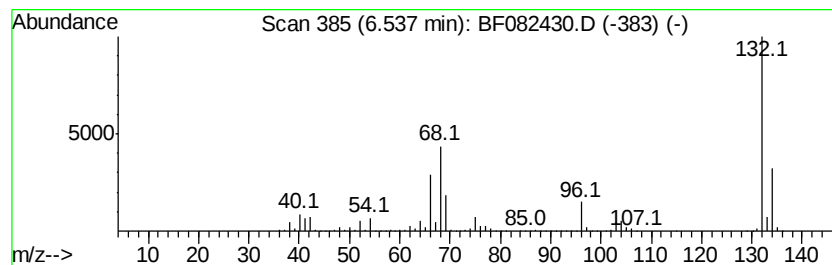
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.54 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.54	94.33 ng	2176170	1,4-Dichlorobenzene-d4	6.77

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-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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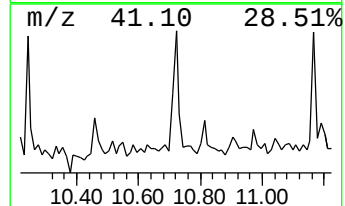
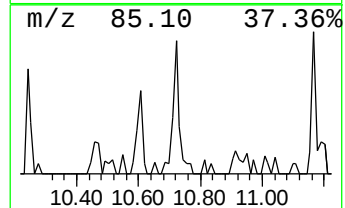
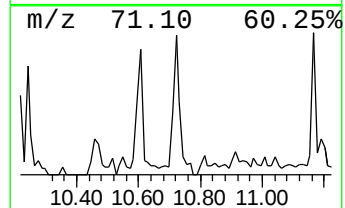
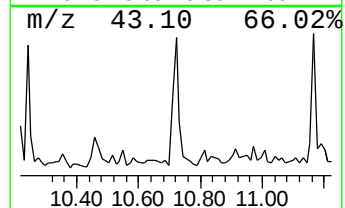
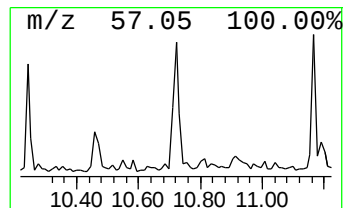
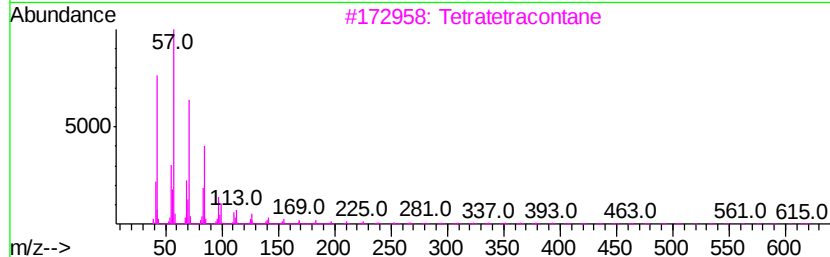
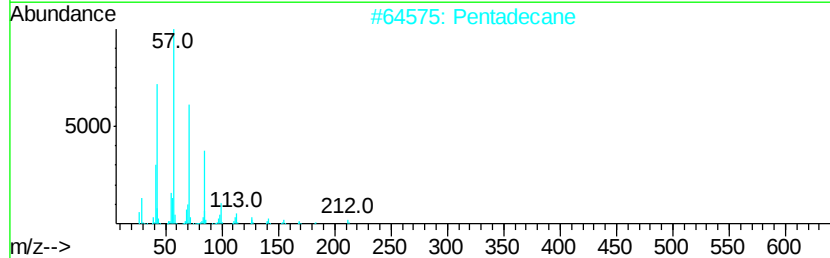
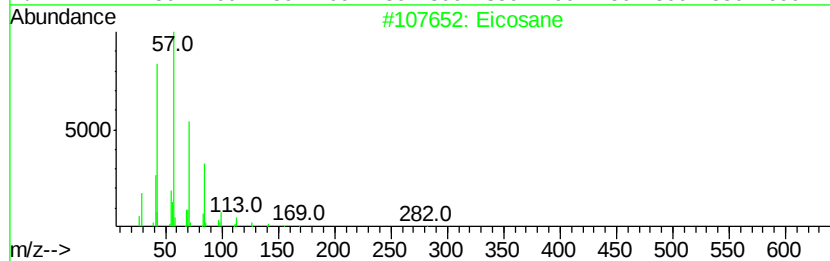
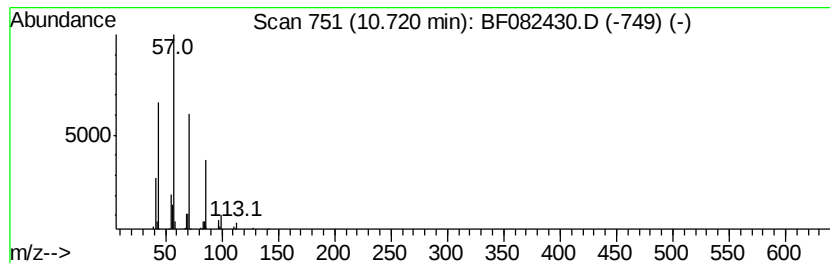
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Eicosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.72	2.29 ng	57088	Phenanthrene-d10	11.30

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	91
2	Pentadecane		212	C15H32	000629-62-9	90
3	Tetratetracontane		619	C44H90	007098-22-8	90
4	Heptacosane		380	C27H56	000593-49-7	90
5	Tetradecane		198	C14H30	000629-59-4	90



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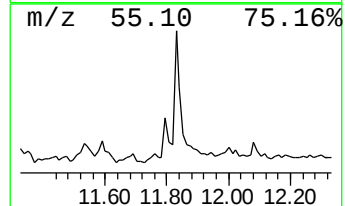
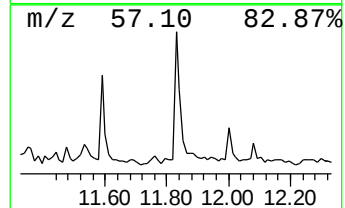
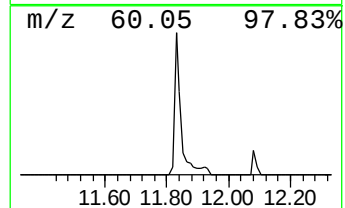
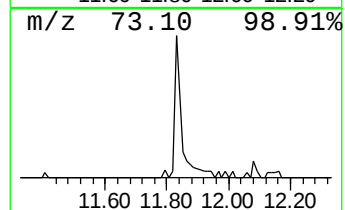
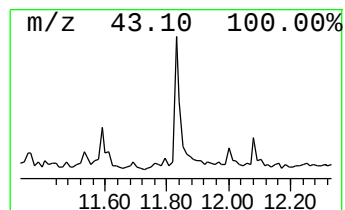
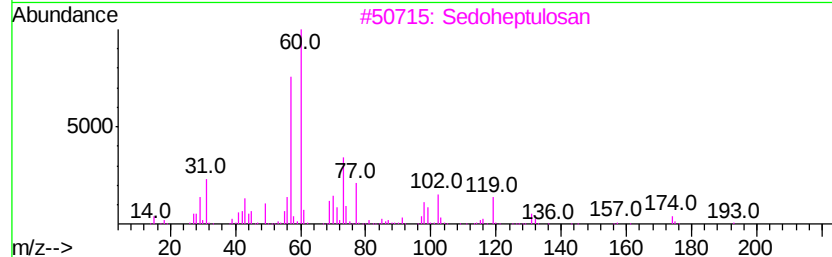
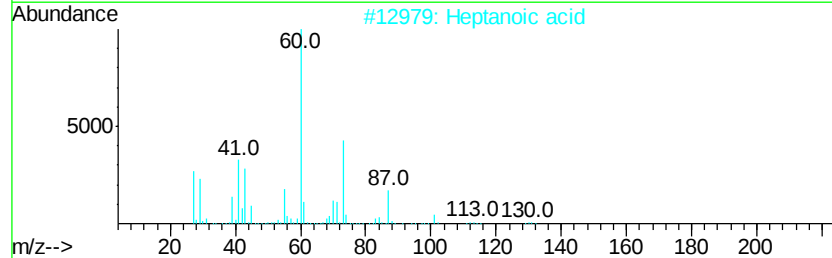
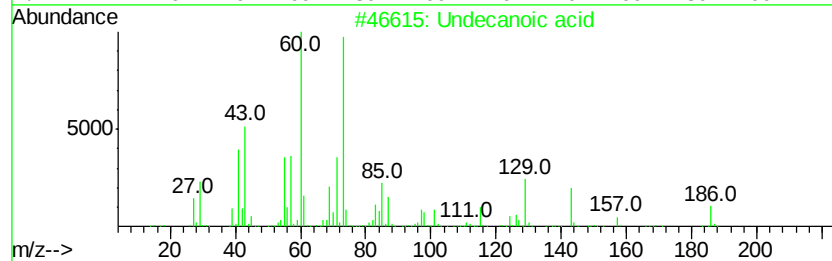
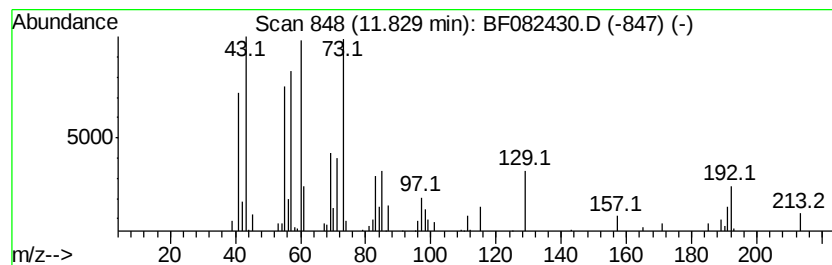
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Undecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.83	4.31 ng	107537	Phenanthrene-d10	11.30

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid		186	C11H22O2	000112-37-8	59
2	Heptanoic acid		130	C7H14O2	000111-14-8	27
3	Sedoheptulosan		192	C7H12O6	000469-90-9	27
4	n-Butyl n-pentyl disulfide		192	C9H20S2	072437-52-6	15
5	1-Tetradecanol, acetate		256	C16H32O2	000638-59-5	11



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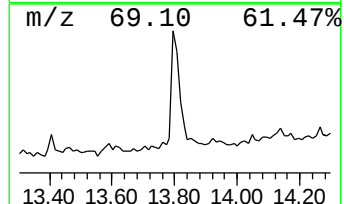
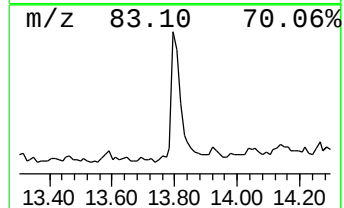
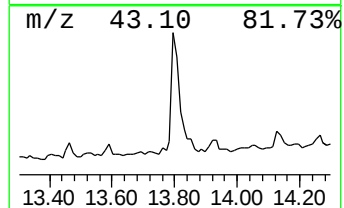
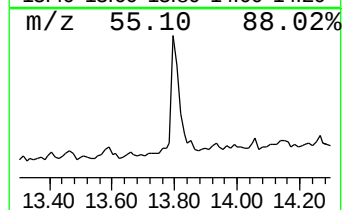
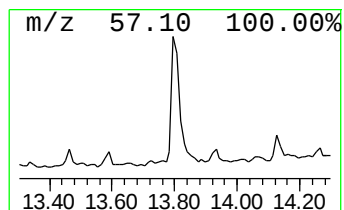
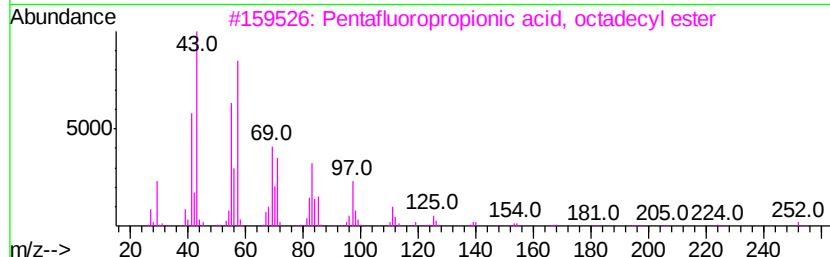
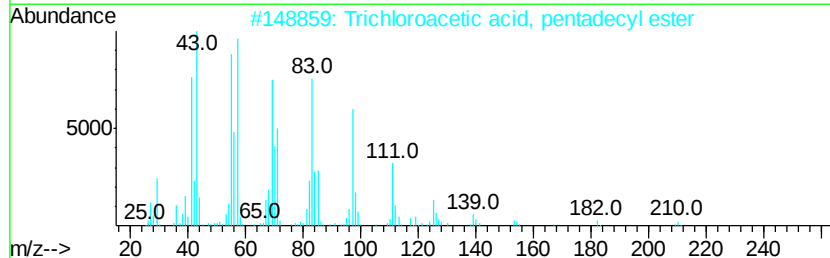
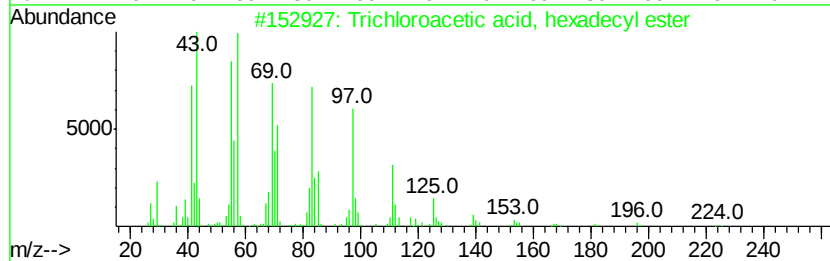
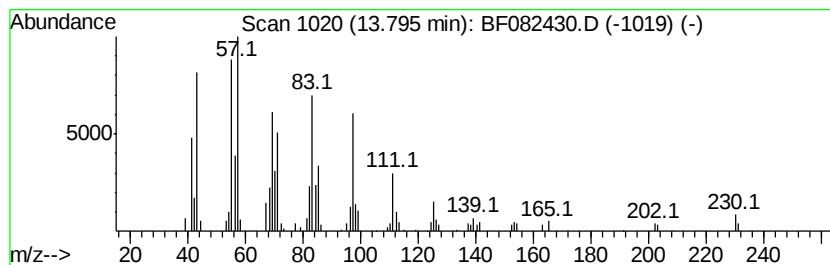
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Trichloroacetic acid, hexad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	6.11 ng	181846	Chrysene-d12	13.96

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	95
2			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
3			Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	91
4			17-Pentatriacontene	491	C35H70	006971-40-0	91
5			Heptafluorobutyric acid, n-penta...	424	C19H31F7O2	1000216-79-3	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102115\
Data File : BF082430.D
Acq On : 22 Oct 2015 4:37
Operator : UM/IZ
Sample : G4116-11
Misc :
ALS Vial : 29 Sample Multiplier: 1

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

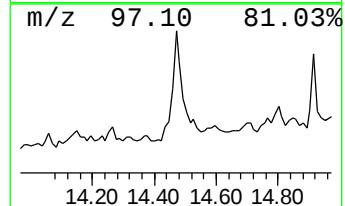
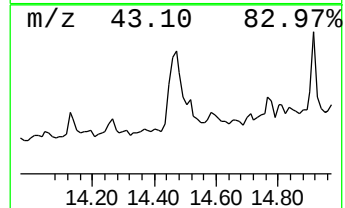
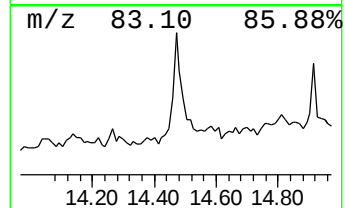
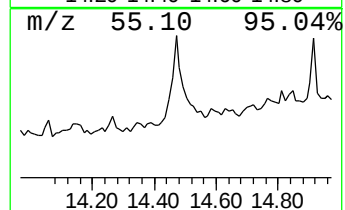
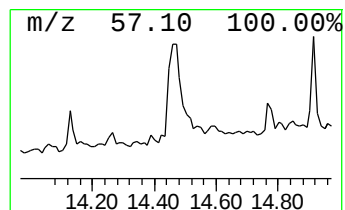
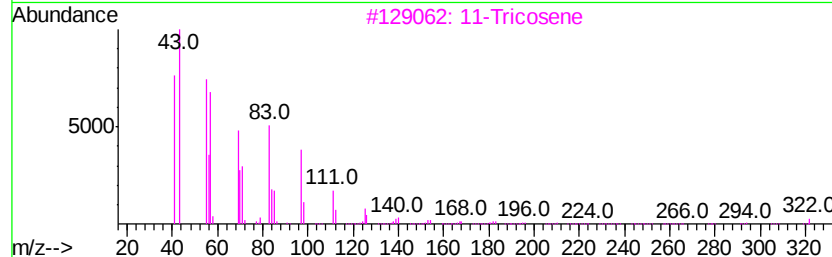
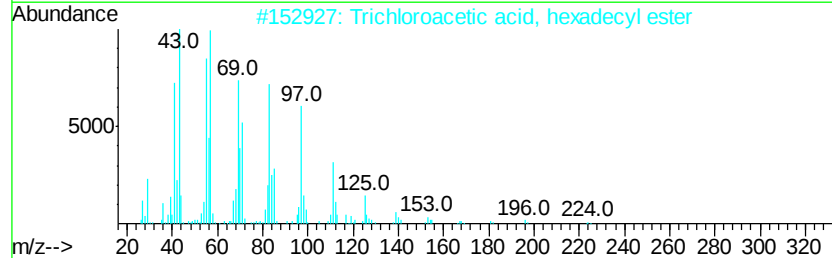
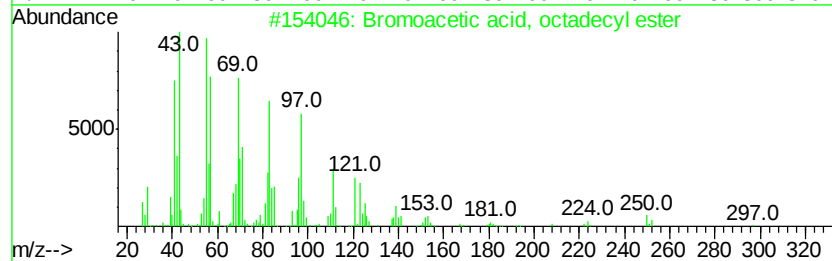
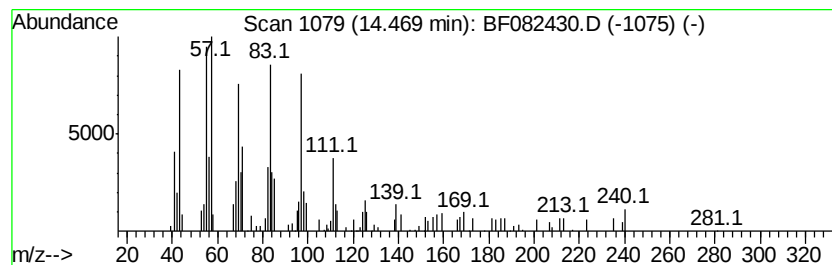
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Bromoacetic acid, octadecyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.47	7.68 ng	228518	Chrysene-d12	13.96

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3		11-Tricosene	322	C23H46	052078-56-5	91
4		1-Nonadecanol	284	C19H40O	001454-84-8	87
5		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	83



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102115\
Data File : BF082430.D
Acq On : 22 Oct 2015 4:37
Operator : UM/IZ
Sample : G4116-11
Misc :
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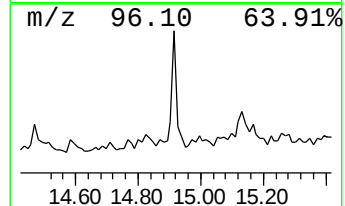
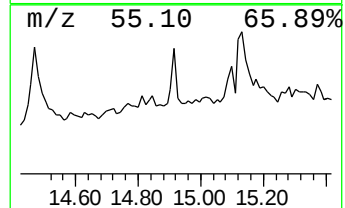
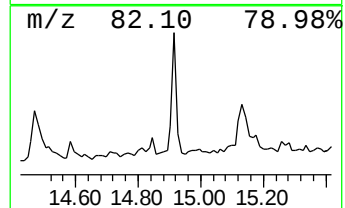
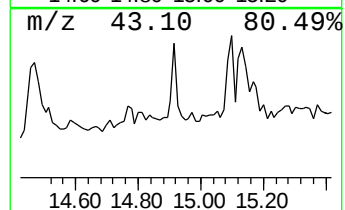
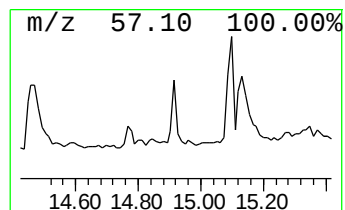
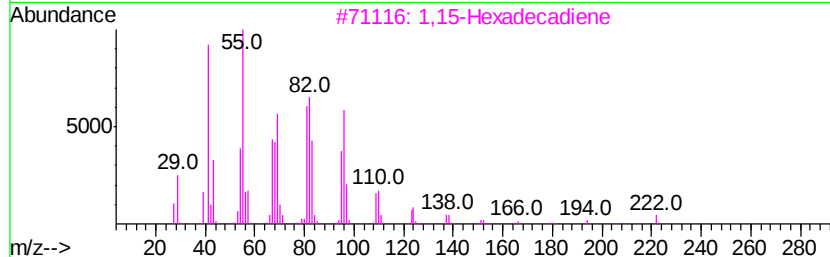
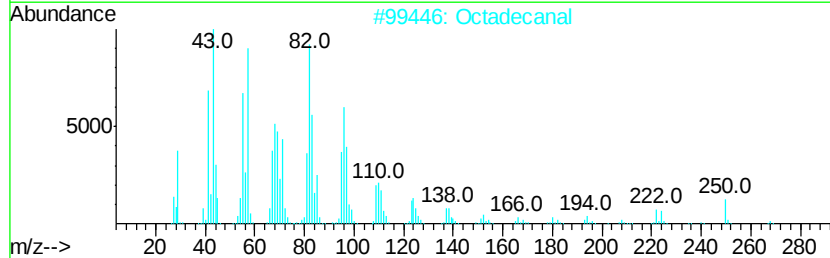
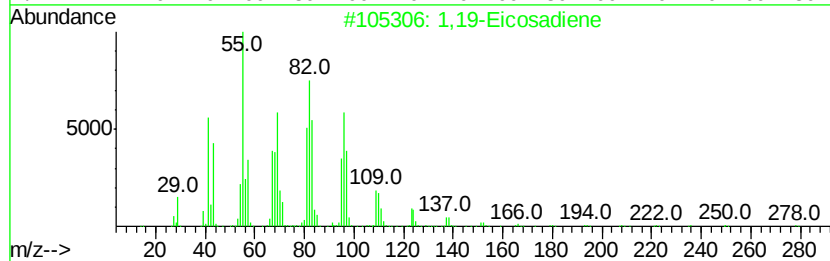
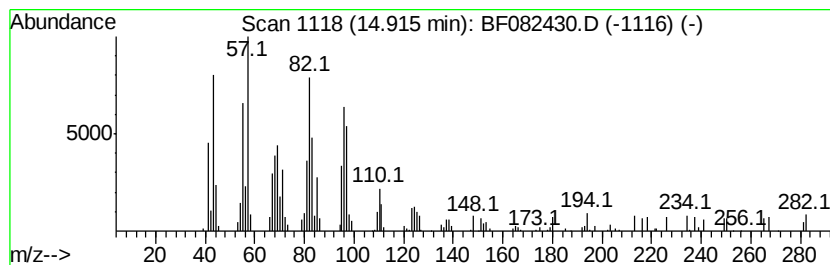
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1,19-Eicosadiene Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.92	2.15 ng	62765	Perylene-d12	15.43	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,19-Eicosadiene	278	C20H38	014811-95-1	90
2	Octadecanal	268	C18H36O	000638-66-4	87
3	1,15-Hexadecadiene	222	C16H30	021964-51-2	83
4	18-Nonadecen-1-ol	282	C19H38O	1000142-89-2	72
5	Oleyl Alcohol	268	C18H36O	000143-28-2	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102115\
Data File : BF082430.D
Acq On : 22 Oct 2015 4:37
Operator : UM/IZ
Sample : G4116-11
Misc :
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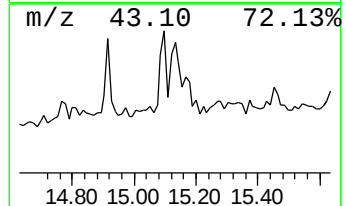
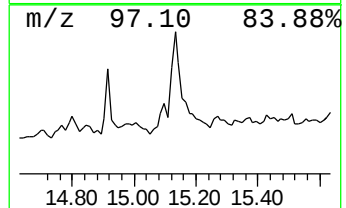
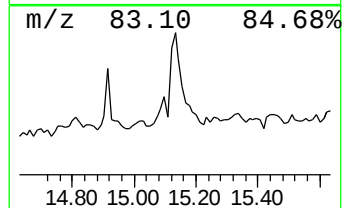
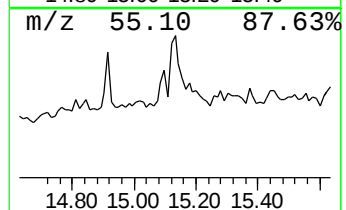
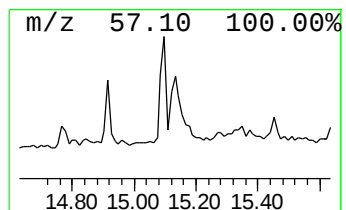
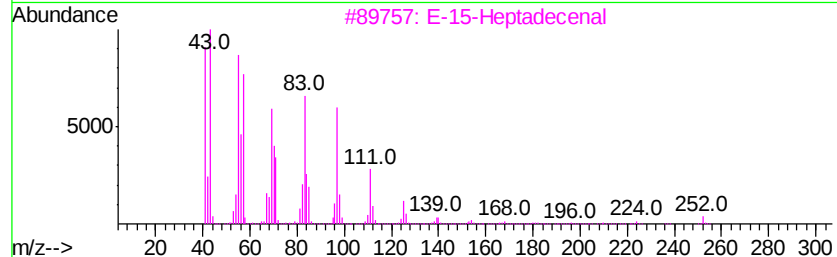
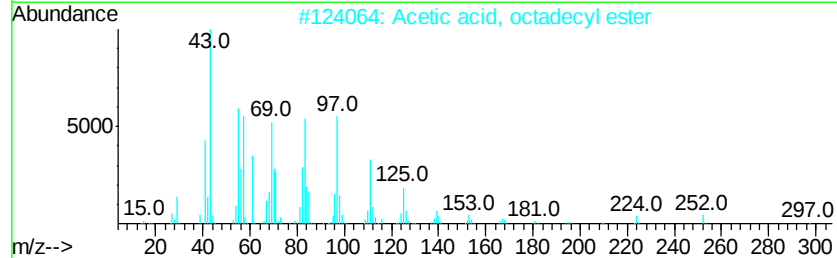
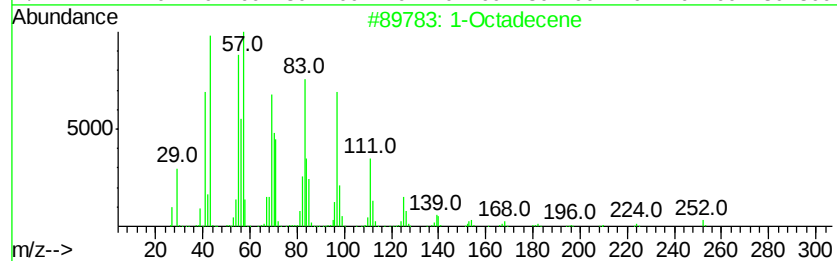
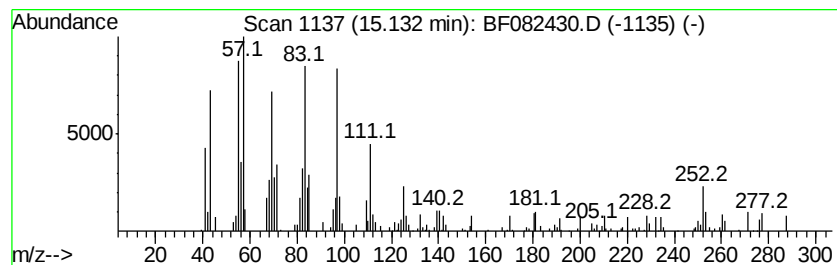
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-Octadecene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.13	4.66 ng	135939	Perylene-d12	15.43	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecene	252	C18H36	000112-88-9	91
2	Acetic acid, octadecyl ester	312	C20H40O2	000822-23-1	83
3	E-15-Heptadecenal	252	C17H32O	1000130-97-9	83
4	E-7-Octadecene	252	C18H36	1000130-92-0	74
5	17-Pentatriacontene	491	C35H70	006971-40-0	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102115\
Data File : BF082430.D
Acq On : 22 Oct 2015 4:37
Operator : UM/IZ
Sample : G4116-11
Misc :
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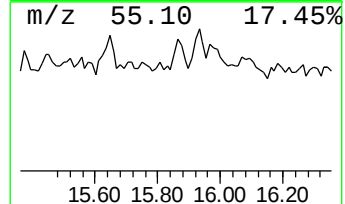
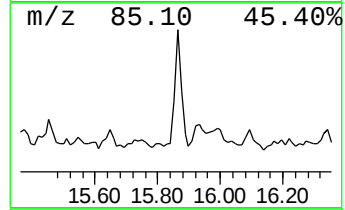
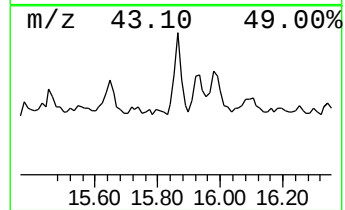
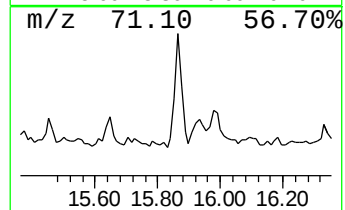
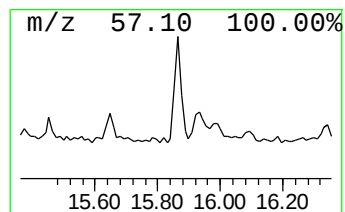
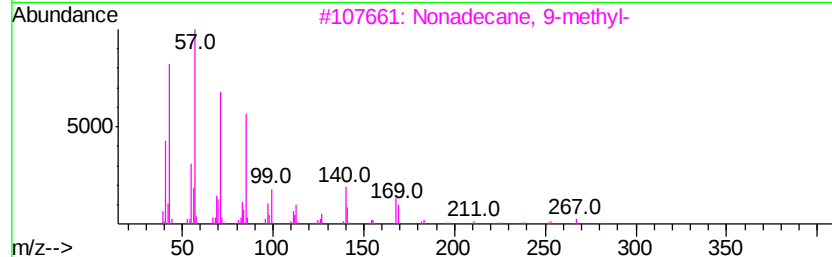
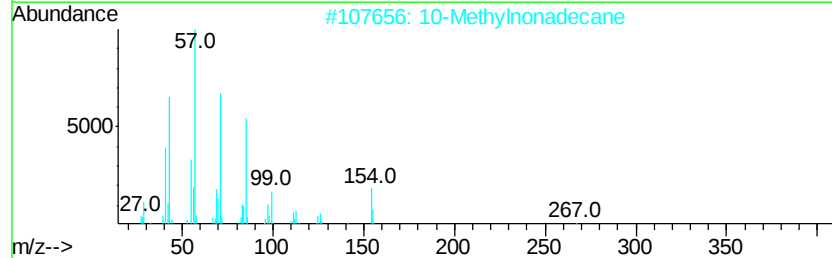
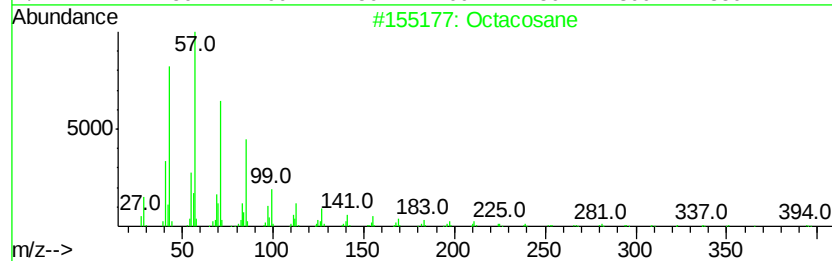
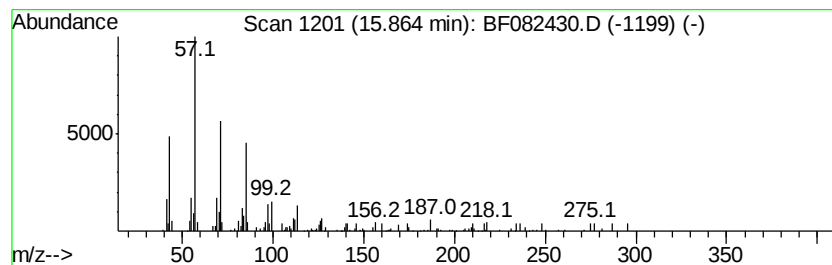
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Octacosane Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.86	2.10 ng	61074	Perylene-d12	15.43
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Octacosane	394 C28H58	000630-02-4	64
2	10-Methylnonadecane	282 C20H42	056862-62-5	58
3	Nonadecane, 9-methyl-	282 C20H42	013287-24-6	58
4	Hexatriacontane	507 C36H74	000630-06-8	58
5	Nonacosane	408 C29H60	000630-03-5	52



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102115\
Data File : BF082430.D
Acq On : 22 Oct 2015 4:37
Operator : UM/IZ
Sample : G4116-11
Misc :
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Instrument :
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ClientSampleId :
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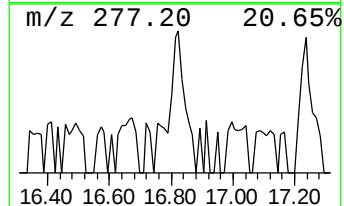
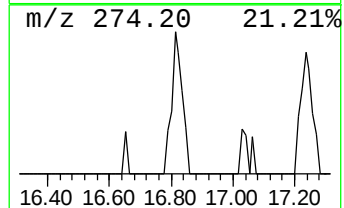
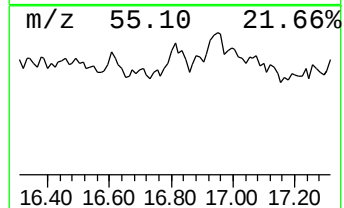
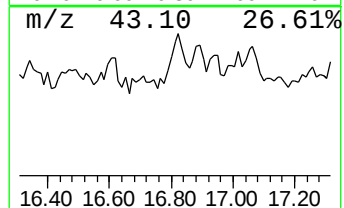
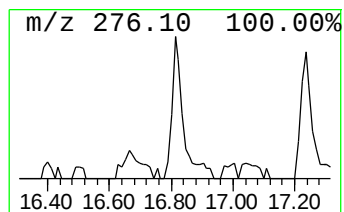
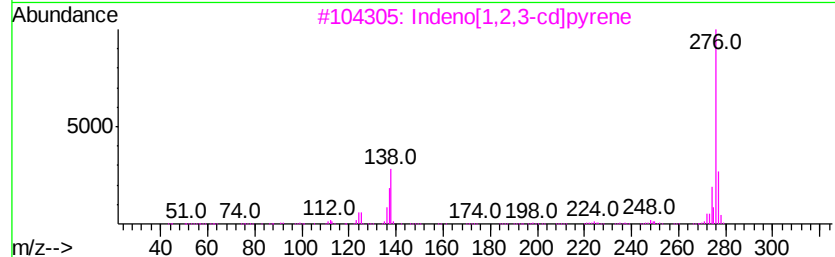
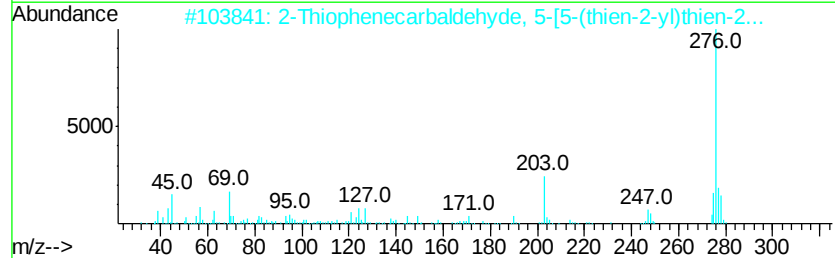
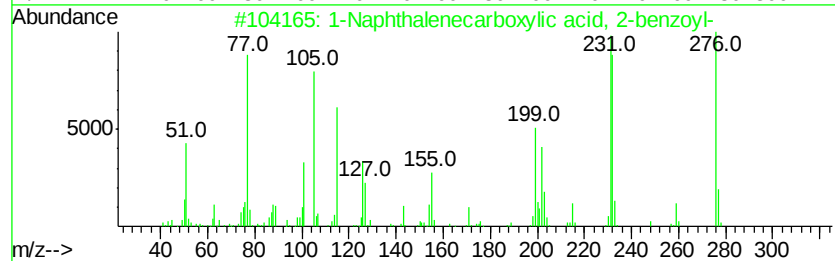
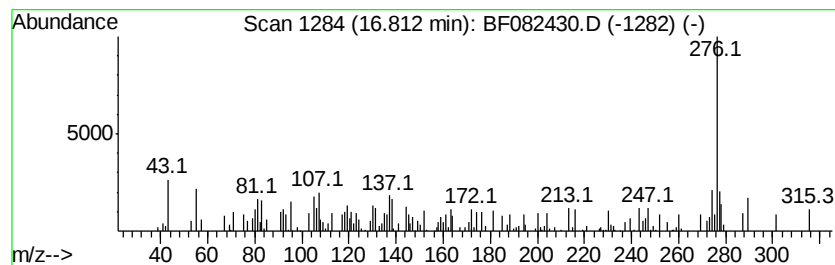
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 1-Naphthalenecarboxylic aci... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.81	2.88 ng	83964	Perylene-d12	15.43

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Naphthalenecarboxylic acid, 2-...	276	C18H12O3	038119-11-8	90
2		2-Thiophenecarbaldehyde, 5-[5-(t...	276	C13H8OS3	1000217-28-5	58
3		Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	55
4		Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	50
5		12H-Benzothieno[2,3-d]pyrido[1,2...	276	C14H16N2S2	102254-63-7	50



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102115\
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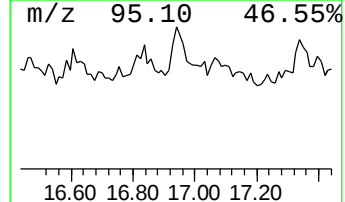
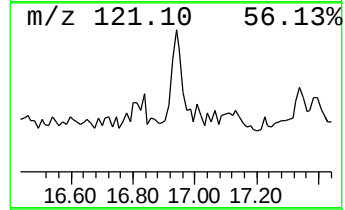
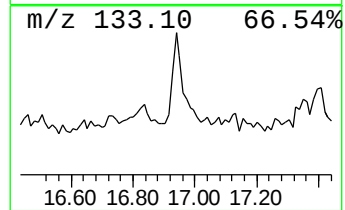
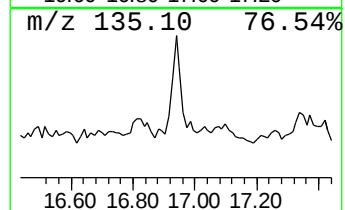
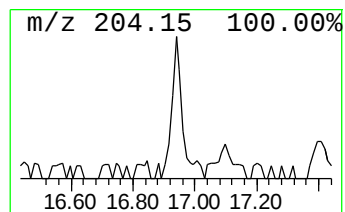
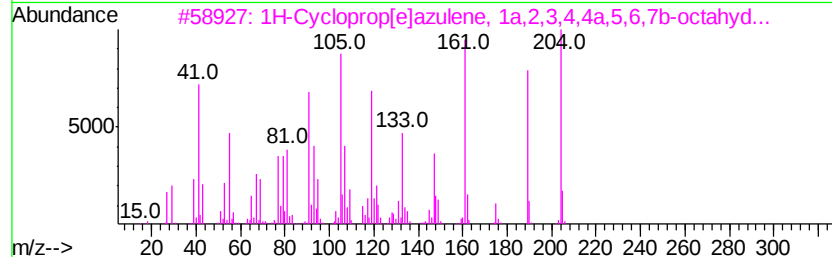
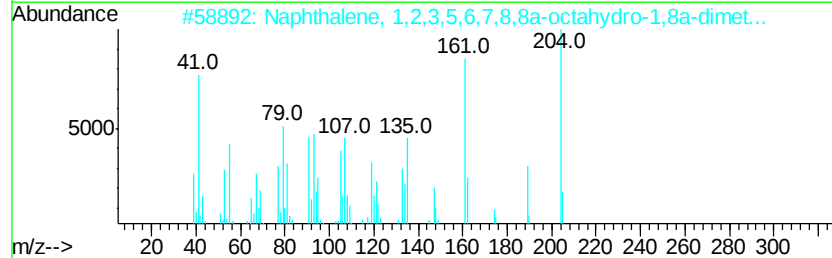
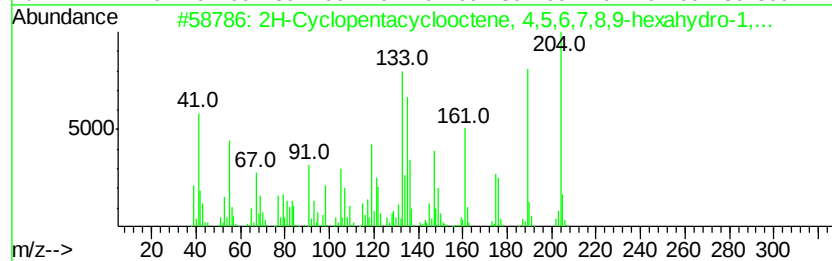
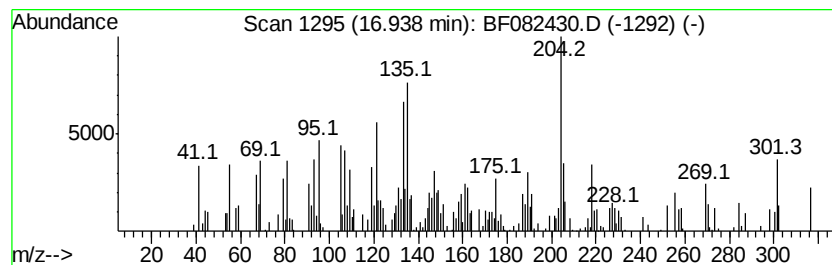
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 2H-Cyclopentacyclooctene, 4... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.94	4.82 ng	140514	Perylene-d12	15.43
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	2H-Cyclopentacyclooctene, 4,5,6,...	204 C15H24	1000221-85-8	60
2	Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204 C15H24	004630-07-3	50
3	1H-Cycloprop[elazulene, 1a,2,3,4...	204 C15H24	000489-40-7	43
4	1,4-Dimethyl-8-isopropylidenetri...	204 C15H24	1000140-07-7	38
5	2-Propenoic acid, 3-bromo-, meth...	164 C4H5BrO2	006214-22-8	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102115\
Data File : BF082430.D
Acq On : 22 Oct 2015 4:37
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Misc :
ALS Vial : 29 Sample Multiplier: 1

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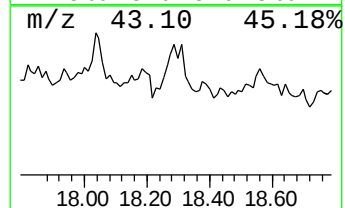
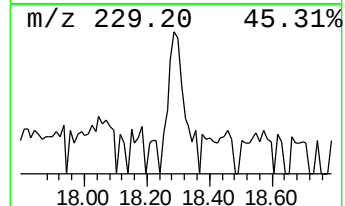
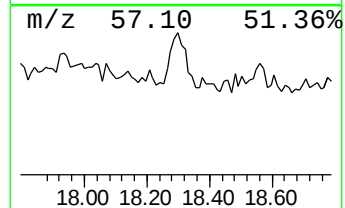
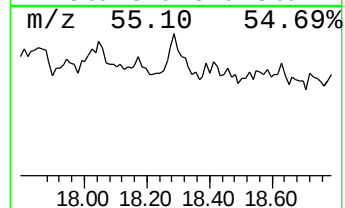
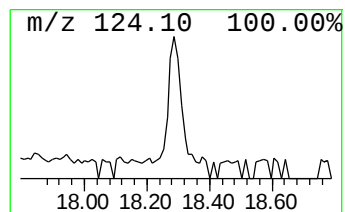
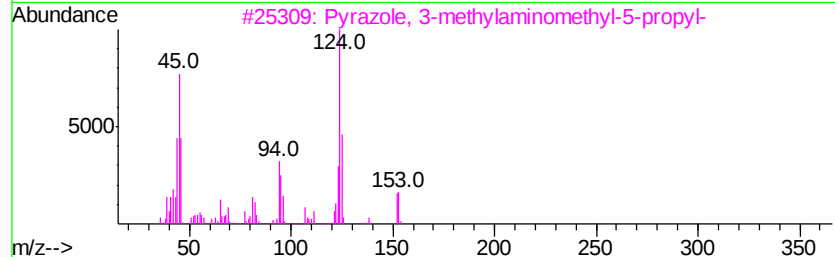
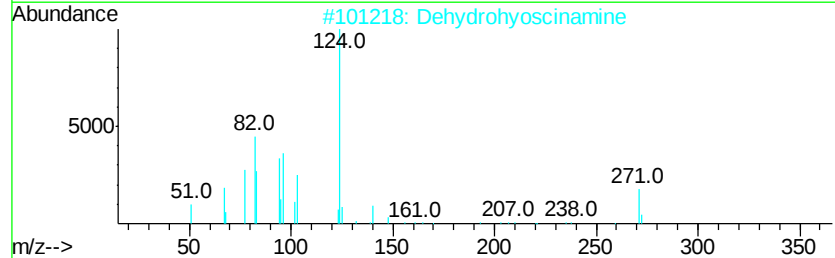
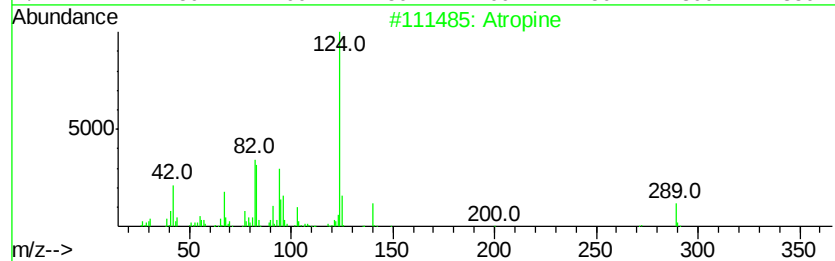
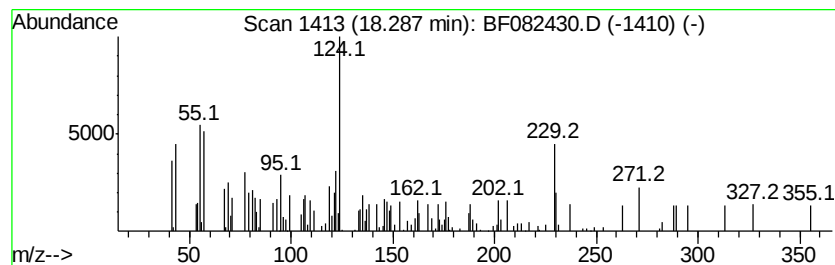
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 unknown18.29 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.29	3.49 ng	101798	Perylene-d12	15.43

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Atropine	289	C17H23NO3	000051-55-8	27
2		Dehydrohyoscinamine	271	C17H21NO2	1000123-19-8	25
3		Pvrazole, 3-methylaminomethyl-5-...	153	C8H15N3	1000262-50-0	25
4		Pvridine, 1-(chloroacetyl)-1,2,3...	159	C7H10ClNO	063177-40-2	22
5		2-Amino-6-methoxypyridine	124	C6H8N2O	017920-35-3	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102115\
Data File : BF082430.D
Acq On : 22 Oct 2015 4:37
Operator : UM/IZ
Sample : G4116-11
Misc :
ALS Vial : 29 Sample Multiplier: 1

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

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.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...	4.94	63.1	ng	1456410	1	6.77	461409	20.0
unknown6.54	6.54	94.3	ng	2176170	1	6.77	461409	20.0
Eicosane	10.72	2.3	ng	57088	4	11.30	498752	20.0
Undecanoic acid	11.83	4.3	ng	107537	4	11.30	498752	20.0
Trichloroacetic a...	13.80	6.1	ng	181846	5	13.96	595235	20.0
Bromoacetic acid,...	14.47	7.7	ng	228518	5	13.96	595235	20.0
1,19-Eicosadiene	14.92	2.1	ng	62765	6	15.43	582936	20.0
1-Octadecene	15.13	4.7	ng	135939	6	15.43	582936	20.0
Octacosane	15.86	2.1	ng	61074	6	15.43	582936	20.0
1-Naphthalenecarb...	16.81	2.9	ng	83964	6	15.43	582936	20.0
2H-Cyclopentacycl...	16.94	4.8	ng	140514	6	15.43	582936	20.0
unknown18.29	18.29	3.5	ng	101798	6	15.43	582936	20.0