

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102315\
 Data File : BF082500.D
 Acq On : 24 Oct 2015 8:41
 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	4.926	240	244	257	rVB	925377	1514820	58.19%	6.357%
2	5.360	280	282	284	rBV	2298531	2378512	91.38%	9.982%
3	5.749	314	316	319	rVB	32029	29686	1.14%	0.125%
4	6.412	371	374	376	rBV	2146960	2406056	92.43%	10.097%
5	6.526	382	384	387	rBV	2501806	2403181	92.32%	10.085%
6	6.755	402	404	406	rBV	545278	491482	18.88%	2.063%
7	6.915	415	418	420	rBV	1469604	1994201	76.61%	8.369%
8	7.326	452	454	457	rBV	1344167	1413614	54.31%	5.932%
9	8.046	514	517	519	rBV	548931	614935	23.62%	2.581%
10	9.120	609	611	614	rBV	2163147	2603022	100.00%	10.924%
11	9.521	644	646	649	rBV	546716	471148	18.10%	1.977%
12	9.795	668	670	673	rBV	583620	678299	26.06%	2.847%
13	10.229	707	708	710	rVB	50290	36272	1.39%	0.152%
14	10.595	737	740	742	rBV	1461999	1445718	55.54%	6.067%
15	10.698	748	749	756	rVB	51796	81627	3.14%	0.343%
16	11.155	787	789	790	rBV	40417	43722	1.68%	0.183%
17	11.281	798	800	803	rBV	430903	618634	23.77%	2.596%
18	11.578	825	826	829	rVB2	28928	27020	1.04%	0.113%
19	11.818	846	847	853	rBV2	96345	113550	4.36%	0.477%
20	12.504	904	907	909	rBV	67430	70543	2.71%	0.296%
21	12.732	923	927	930	rBV	60864	71555	2.75%	0.300%
22	12.881	937	940	942	rBV	1985490	1899141	72.96%	7.970%
23	13.109	958	960	964	rBV3	14884	36615	1.41%	0.154%
24	13.418	984	987	989	rVB2	24765	32641	1.25%	0.137%
25	13.841	1020	1024	1031	rBV2	69718	196041	7.53%	0.823%
26	13.978	1033	1036	1038	rBV	438785	549743	21.12%	2.307%
27	14.492	1079	1081	1083	rBV2	24945	44454	1.71%	0.187%
28	14.550	1083	1086	1090	rVV3	44249	121823	4.68%	0.511%
29	14.904	1115	1117	1119	rBV	35951	51580	1.98%	0.216%
30	14.984	1122	1124	1127	rBV	47156	58738	2.26%	0.247%
31	15.087	1131	1133	1137	rVV	31672	68260	2.62%	0.286%
32	15.167	1138	1140	1144	rVV2	42114	62924	2.42%	0.264%
33	15.235	1144	1146	1150	rBV2	48342	126392	4.86%	0.530%
34	15.441	1162	1164	1166	rVB	24677	29770	1.14%	0.125%

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BT-01(0-2)

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	15.498	1166	1169	1176	rVB	414715	541272	20.79%	2.272%
36	15.944	1206	1208	1212	rBV	43637	70502	2.71%	0.296%
37	17.007	1299	1301	1304	rVB3	67683	115125	4.42%	0.483%
38	17.464	1337	1341	1347	rBV6	57187	180721	6.94%	0.758%
39	18.367	1416	1420	1428	rVB5	37175	135290	5.20%	0.568%

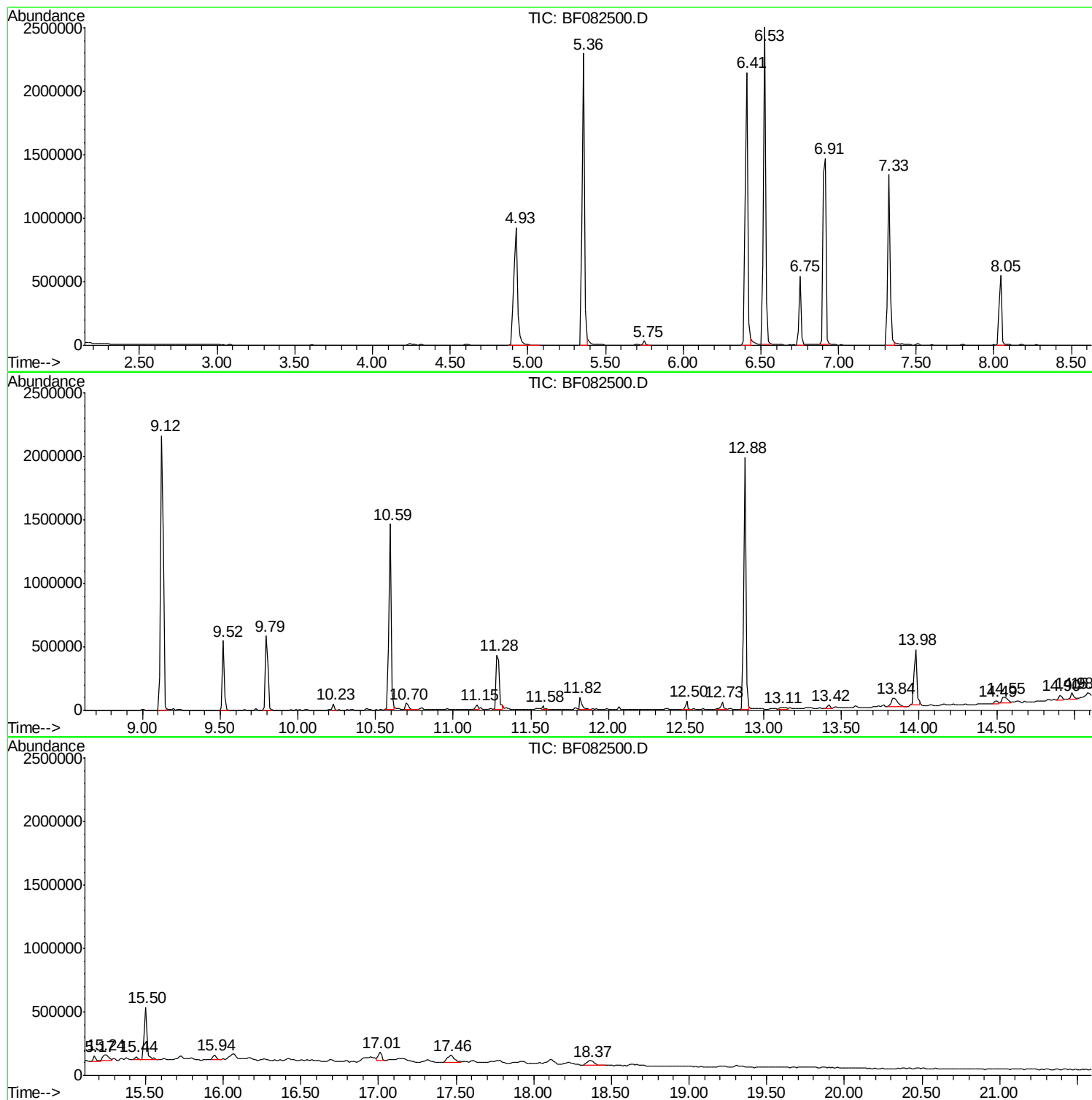
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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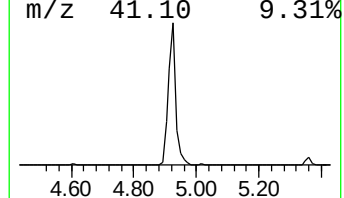
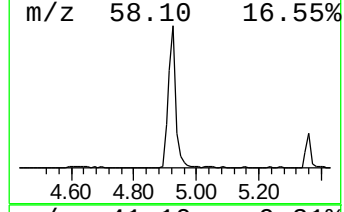
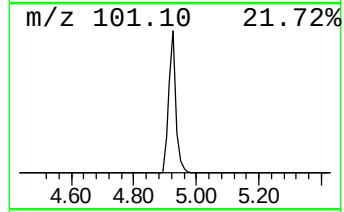
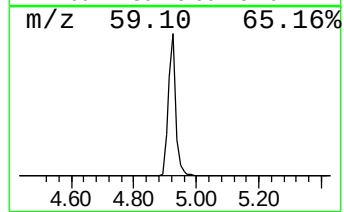
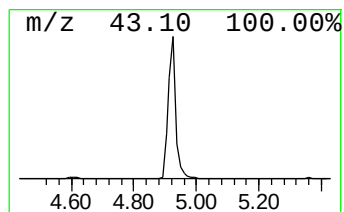
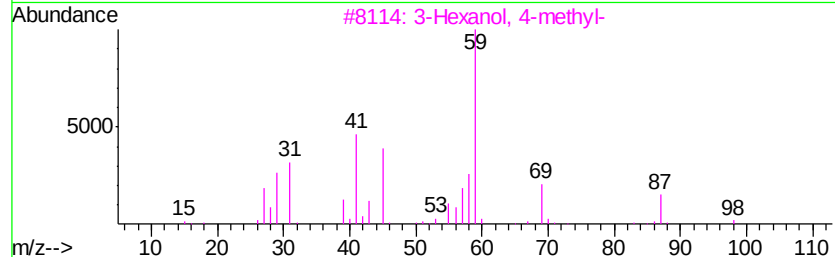
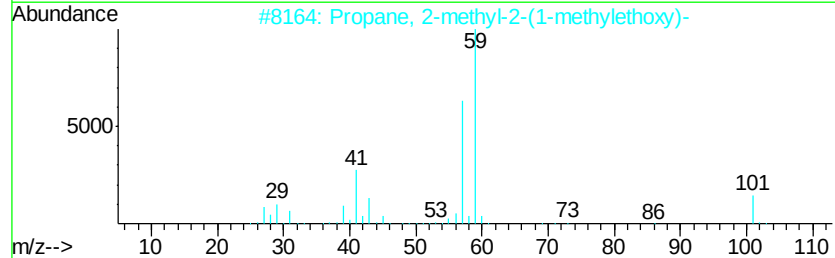
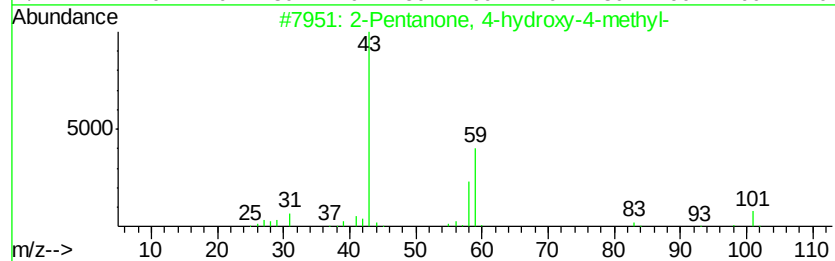
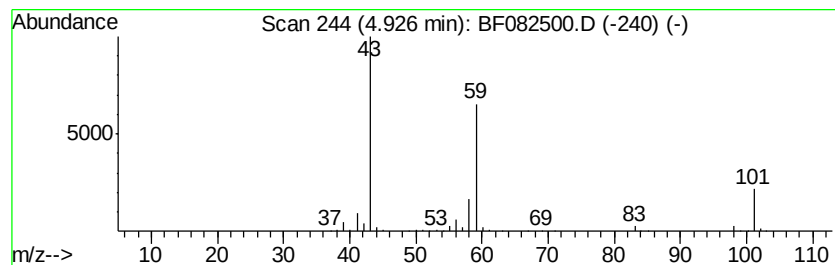
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	61.64 ng	1514820	1,4-Dichlorobenzene-d4	6.75

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5		Acetone	58	C3H6O	000067-64-1	9



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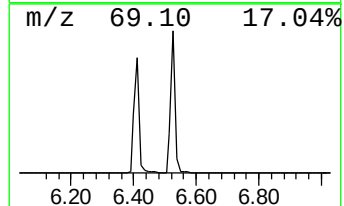
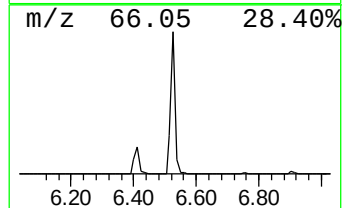
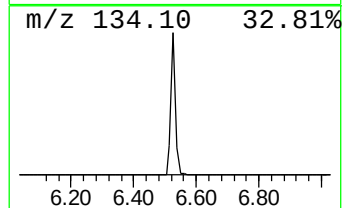
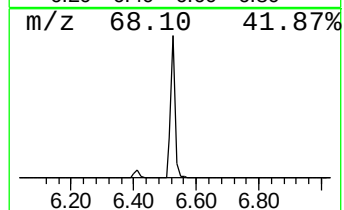
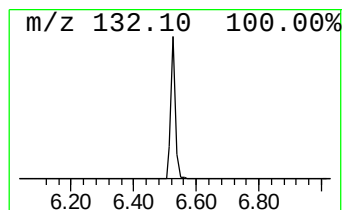
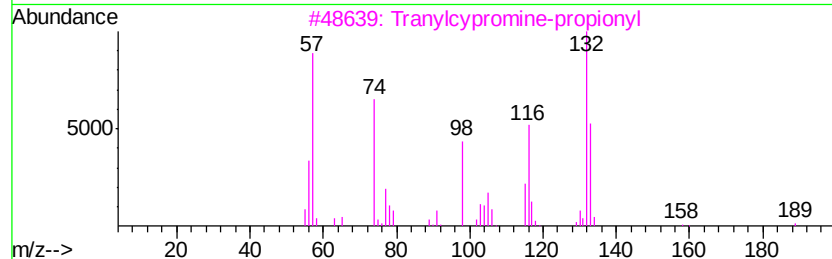
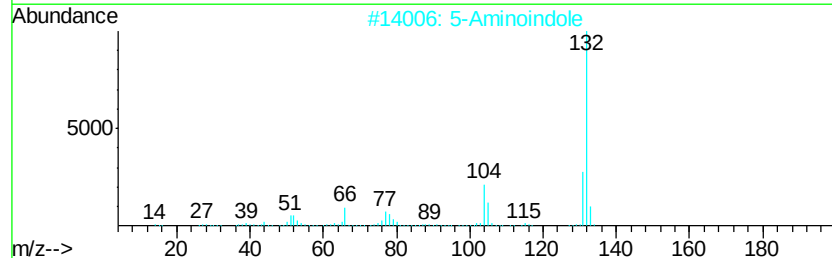
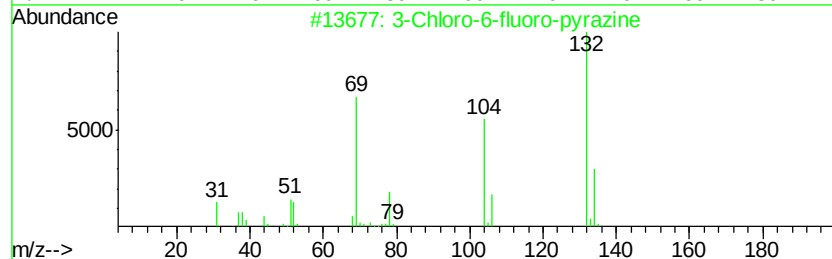
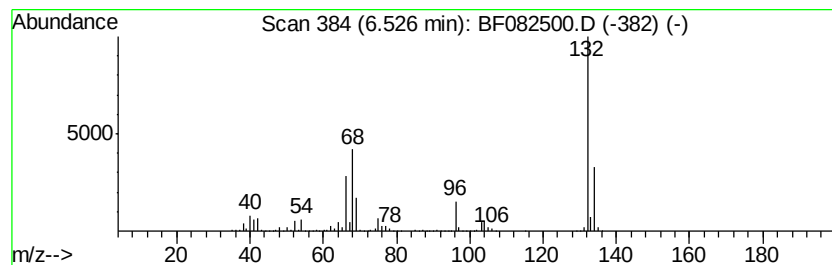
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Peak Number 2 unknown6.53 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.53	97.79 ng	2403180	1,4-Dichlorobenzene-d4	6.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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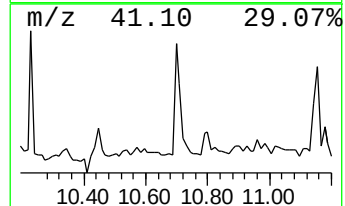
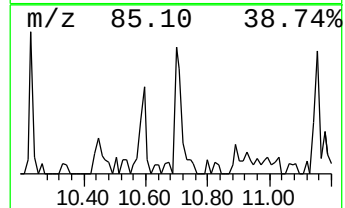
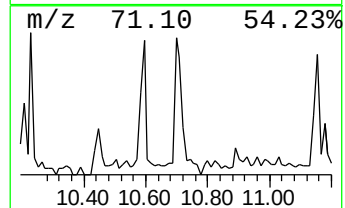
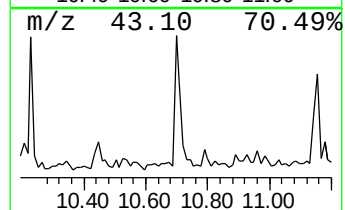
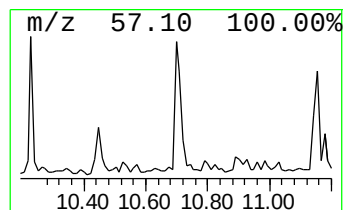
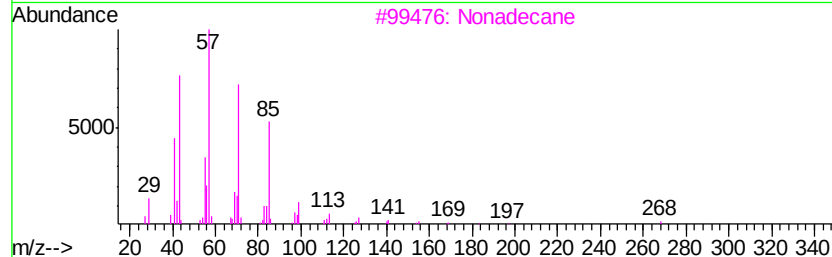
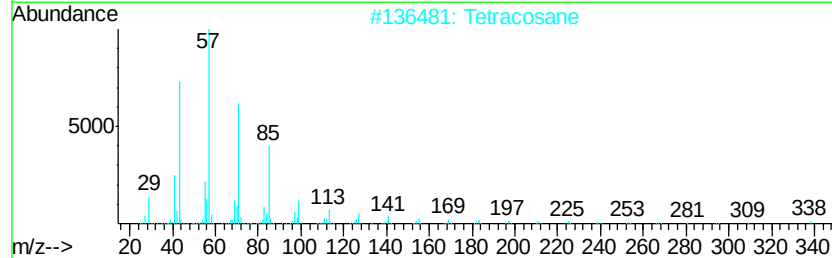
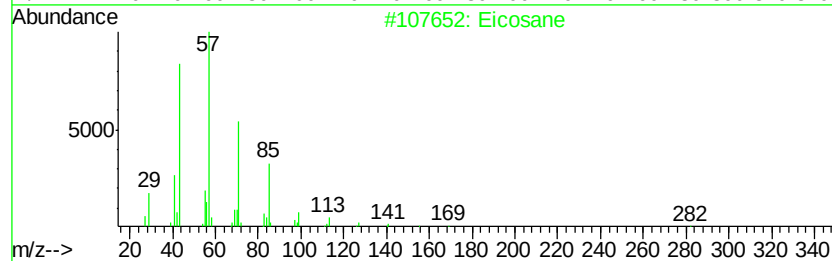
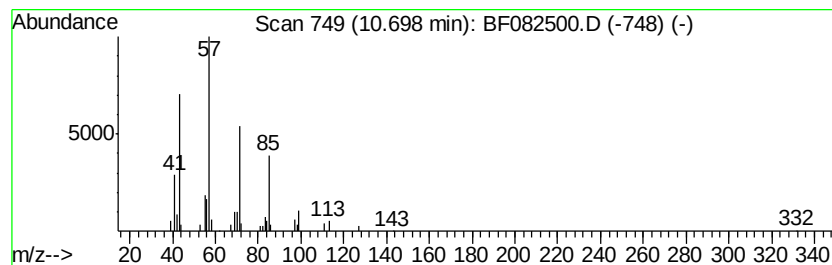
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Eicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.70	2.64 ng	81627	Phenanthrene-d10		11.29
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	Nonadecane	268	C19H40	000629-92-5	87
4	10-Methylnonadecane	282	C20H42	056862-62-5	87
5	Eicosane, 10-methyl-	296	C21H44	054833-23-7	86



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ALS Vial : 29 Sample Multiplier: 1

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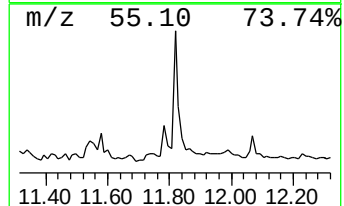
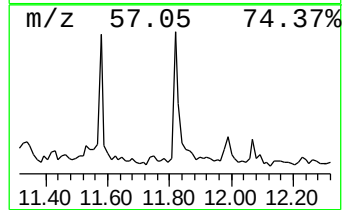
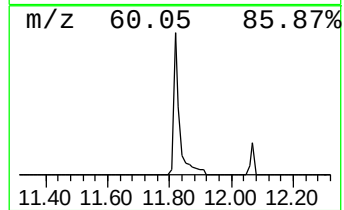
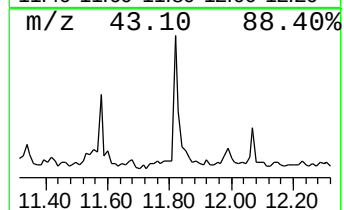
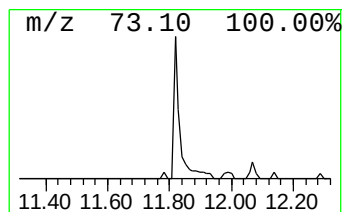
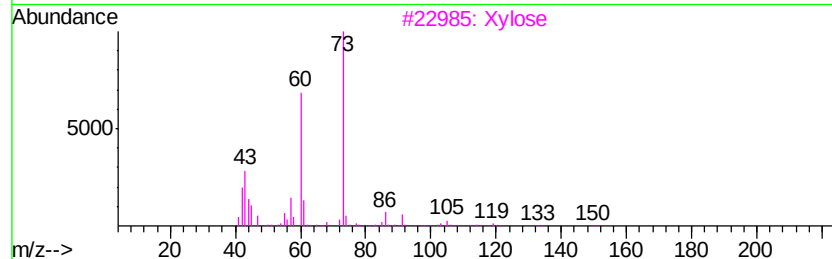
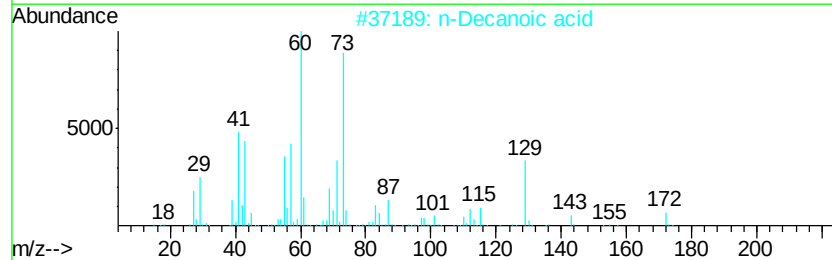
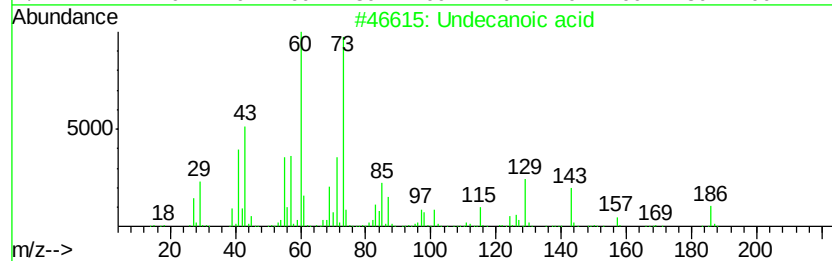
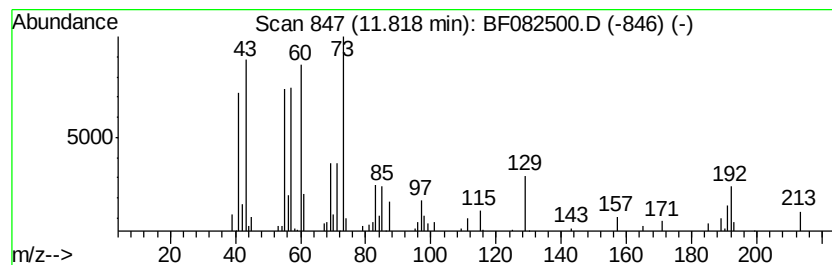
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Undecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.82	3.67 ng	113550	Phenanthrene-d10		11.29

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecanoic acid	186	C11H22O2	000112-37-8	53
2			n-Decanoic acid	172	C10H20O2	000334-48-5	47
3			Xylose	150	C5H10O5	000058-86-6	43
4			Lactose	342	C12H22O11	000063-42-3	38
5			N-(5-Oxo-tetrahydro-furan-2-yl)me...	157	C7H11NO3	1000188-71-2	38



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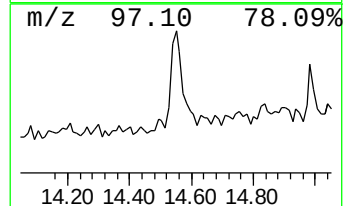
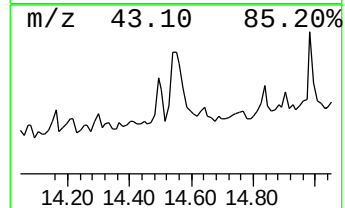
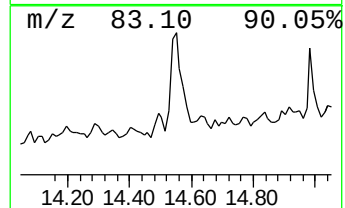
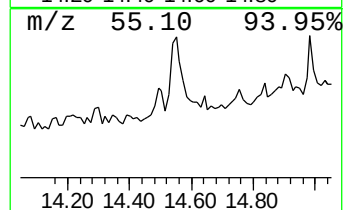
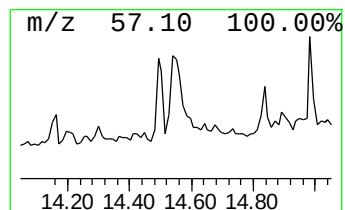
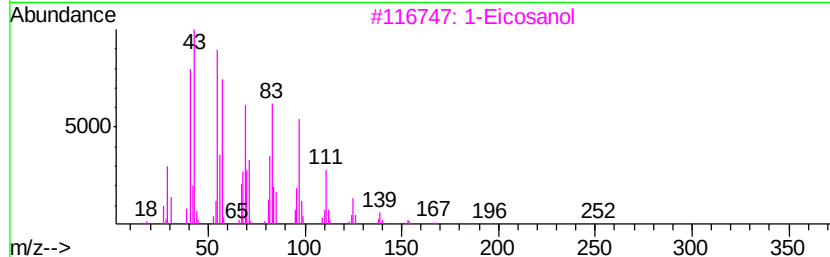
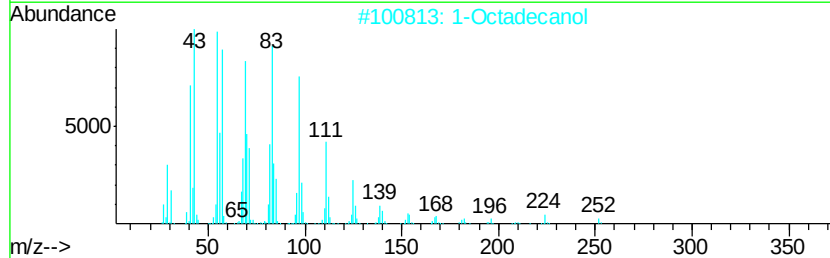
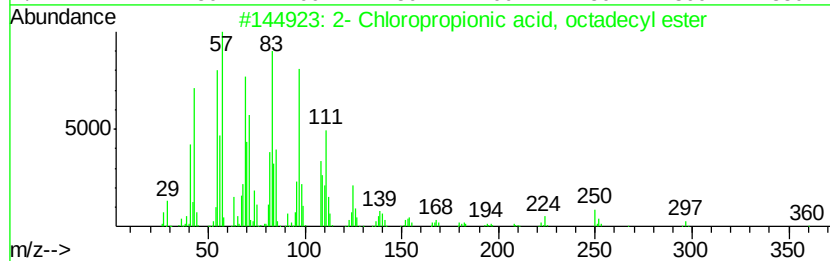
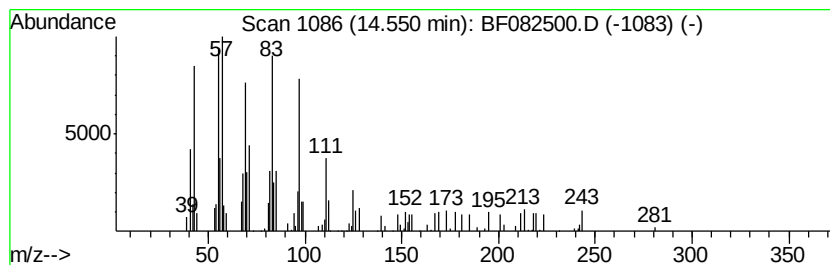
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Peak Number 7 2- Chloropropionic acid, oc... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.55	4.43 ng	121823	Chrysene-d12	13.98		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-	Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91
2	1-Octadecanol		270	C18H38O	000112-92-5	76
3	1-Eicosanol		298	C20H42O	000629-96-9	76
4	Trichloroacetic acid, hexadecyl ...		386	C18H33Cl3O2	074339-54-1	74
5	1-Nonadecanol		284	C19H40O	001454-84-8	74



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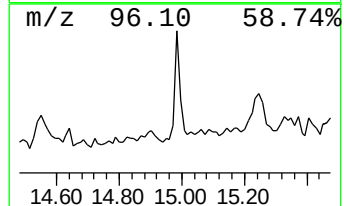
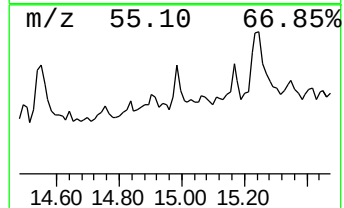
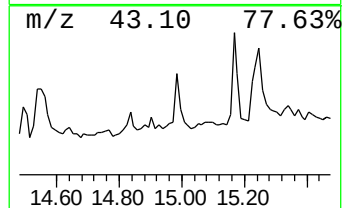
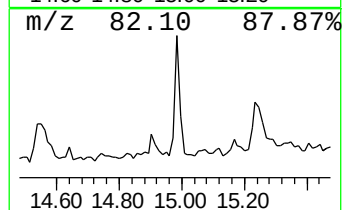
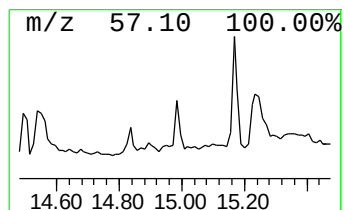
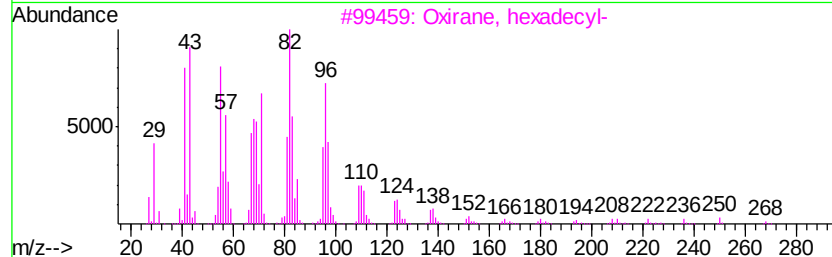
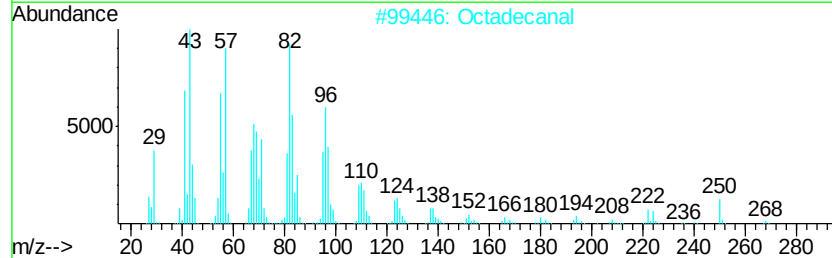
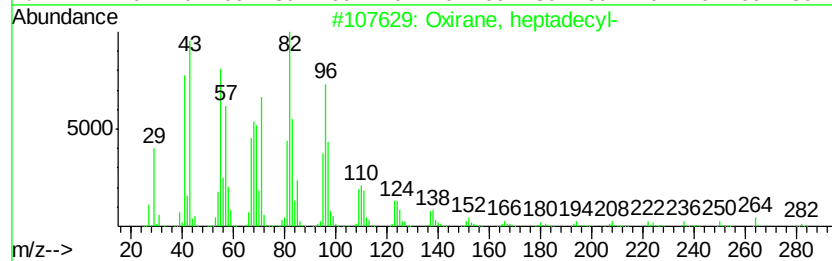
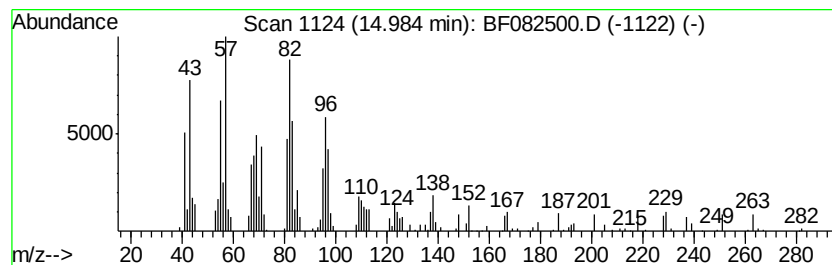
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ClientSampleId :
BT-01(0-2)

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

Peak Number 8 Oxirane, heptadecyl- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.98	2.17 ng	58738	Perylene-d12		15.50
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	93
2	Octadecanal	268	C18H36O	000638-66-4	91
3	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	87
4	Oxirane, tetradecyl-	240	C16H32O	007320-37-8	80
5	13-Octadecenal	266	C18H34O	056554-90-6	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102315\
Data File : BF082500.D
Acq On : 24 Oct 2015 8:41
Operator : UM/IZ
Sample : G4116-11
Misc :
ALS Vial : 29 Sample Multiplier: 1

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

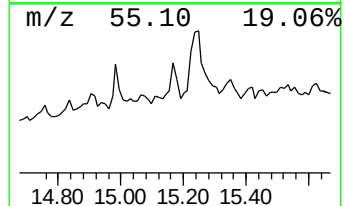
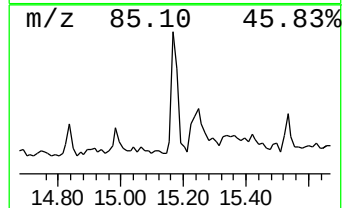
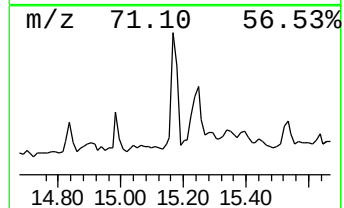
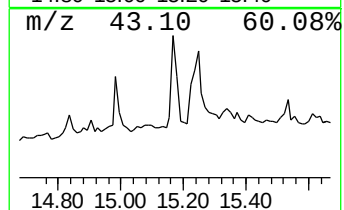
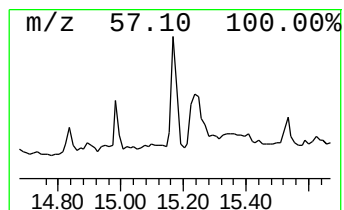
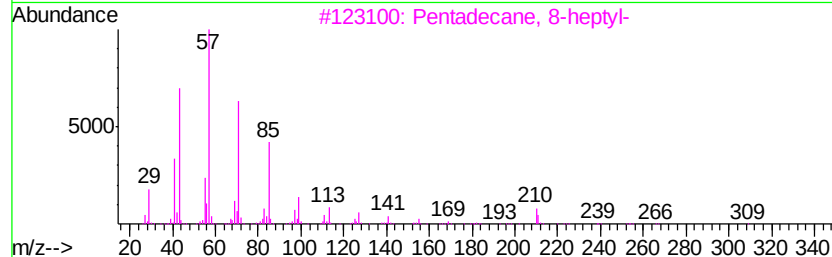
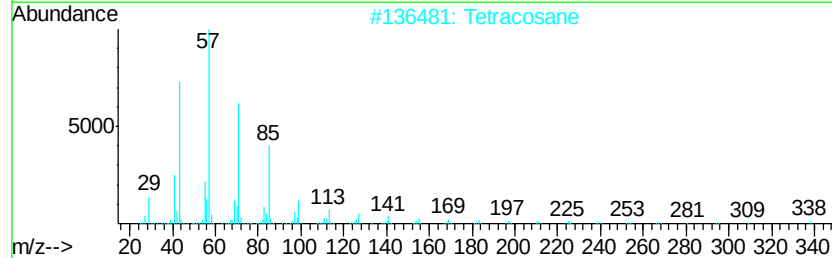
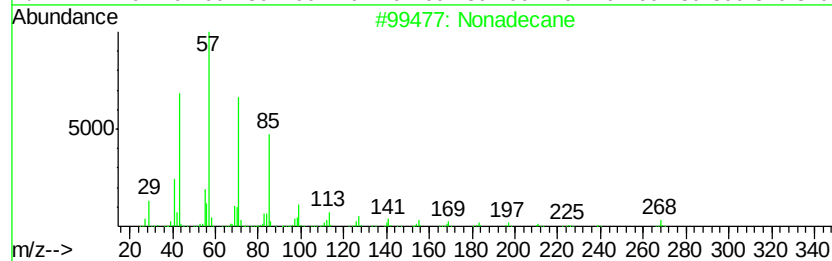
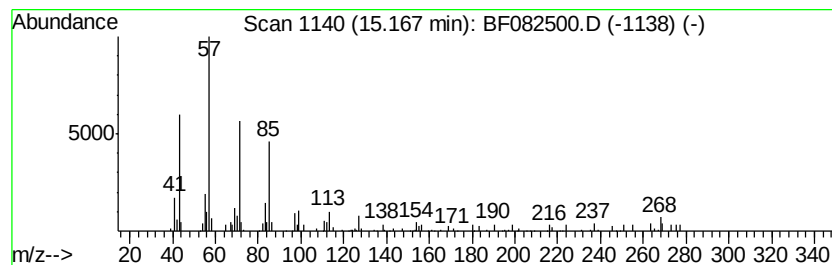
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Nonadecane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.17	2.33 ng	62924	Perylene-d12	15.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecane	268	C19H40	000629-92-5	81
2		Tetracosane	338	C24H50	000646-31-1	68
3		Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	64
4		Heneicosane	296	C21H44	000629-94-7	64
5		Heptadecane	240	C17H36	000629-78-7	59



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102315\
Data File : BF082500.D
Acq On : 24 Oct 2015 8:41
Operator : UM/IZ
Sample : G4116-11
Misc :
ALS Vial : 29 Sample Multiplier: 1

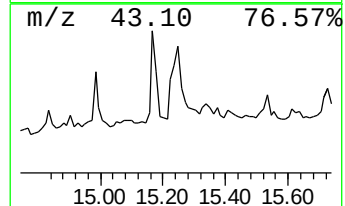
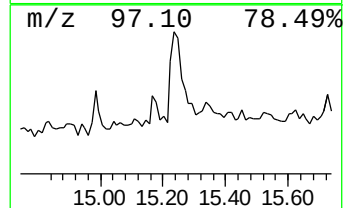
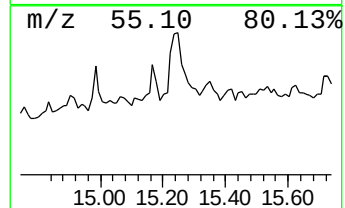
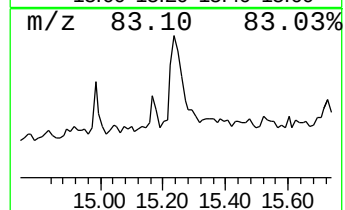
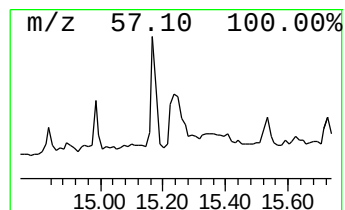
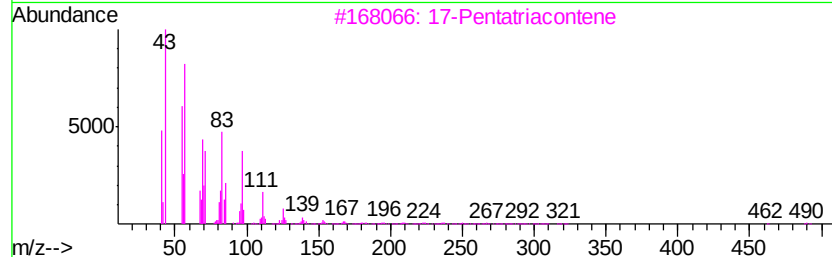
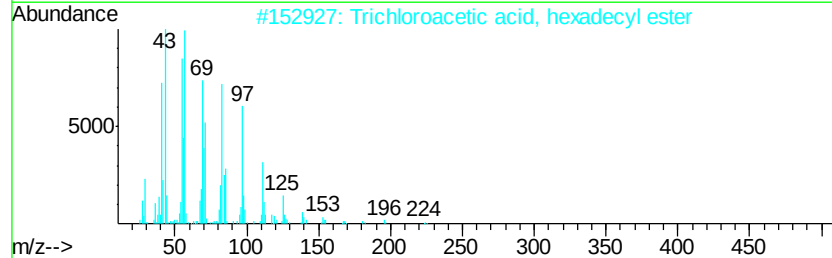
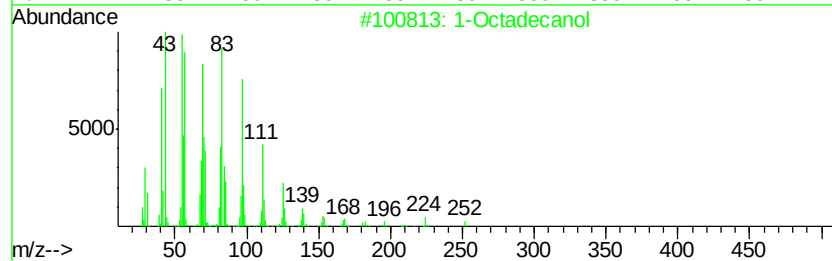
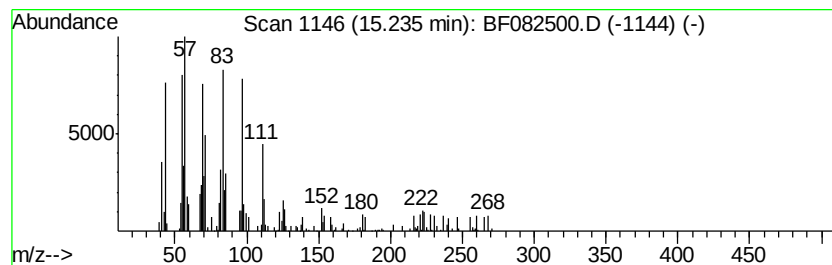
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1-Octadecanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.24	4.67 ng	126392	Perylene-d12	15.50
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Octadecanol	270 C18H38O	000112-92-5	70
2	Trichloroacetic acid, hexadecyl ...	386 C18H33Cl3O2	074339-54-1	64
3	17-Pentatriacontene	491 C35H70	006971-40-0	62
4	Dichloroacetic acid, tridecyl ester	310 C15H28Cl2O2	1000280-48-3	62
5	Trichloroacetic acid, pentadecyl...	372 C17H31Cl3O2	074339-53-0	58



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102315\
Data File : BF082500.D
Acq On : 24 Oct 2015 8:41
Operator : UM/IZ
Sample : G4116-11
Misc :
ALS Vial : 29 Sample Multiplier: 1

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

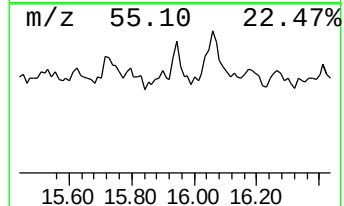
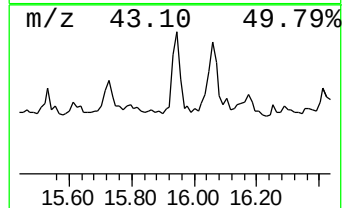
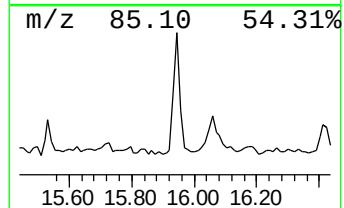
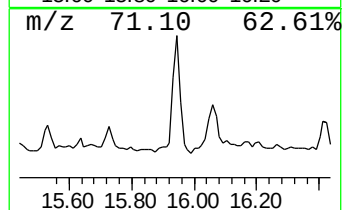
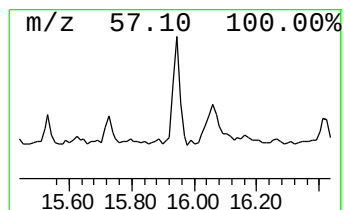
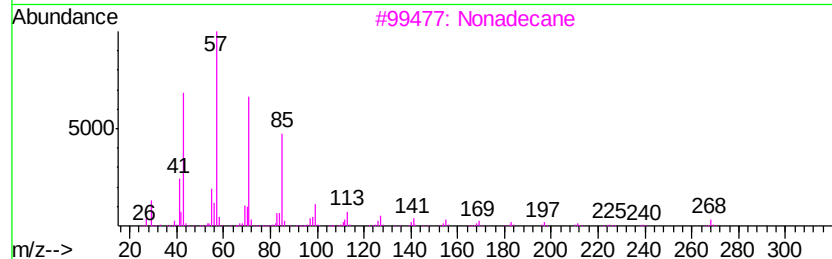
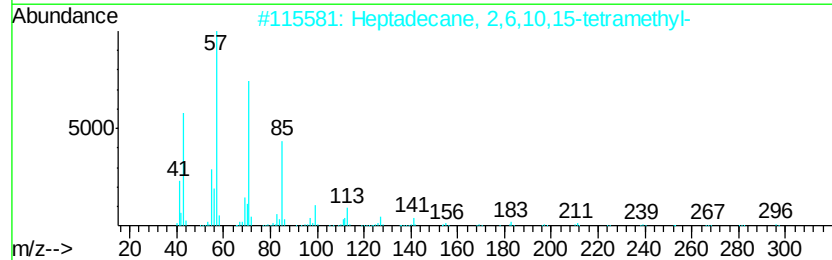
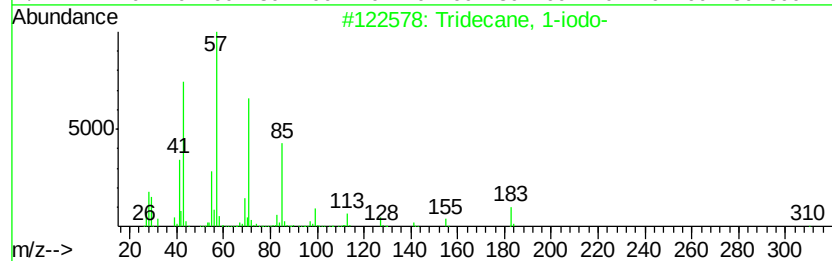
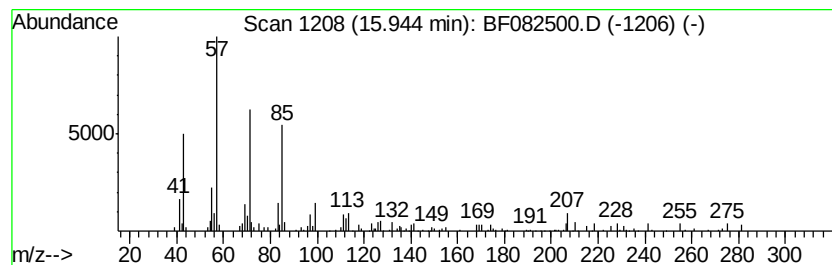
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Tridecane, 1-iodo- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.94	2.61 ng	70502	Perylene-d12	15.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	72
2		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	64
3		Nonadecane	268	C19H40	000629-92-5	64
4		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	64
5		Heptadecane	240	C17H36	000629-78-7	58



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102315\
Data File : BF082500.D
Acq On : 24 Oct 2015 8:41
Operator : UM/IZ
Sample : G4116-11
Misc :
ALS Vial : 29 Sample Multiplier: 1

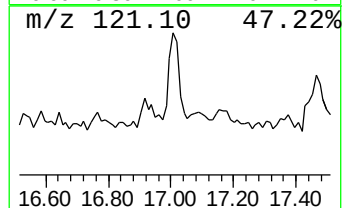
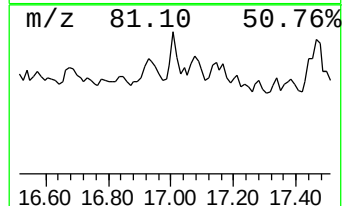
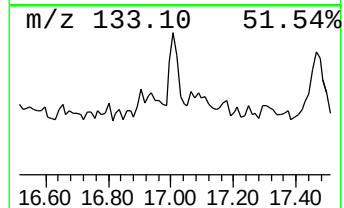
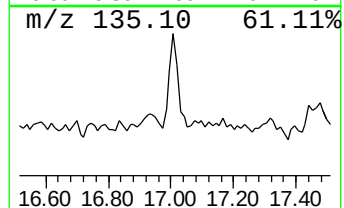
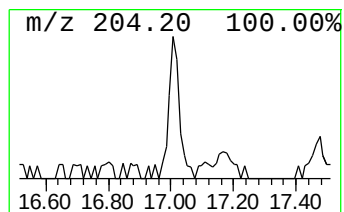
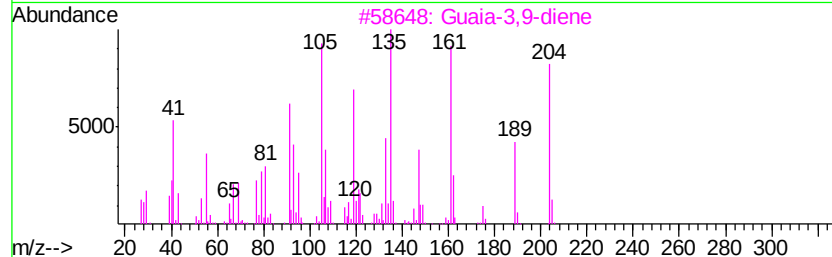
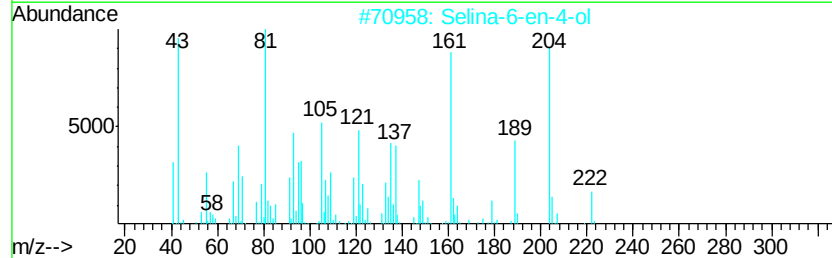
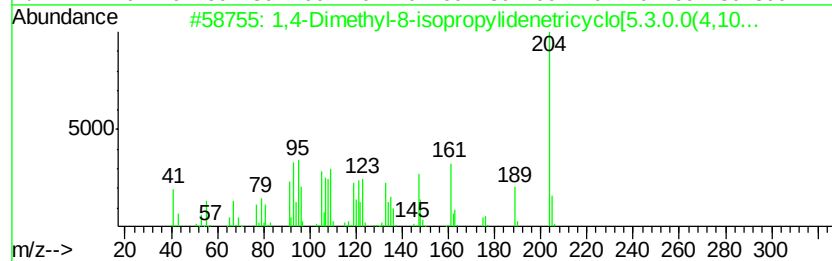
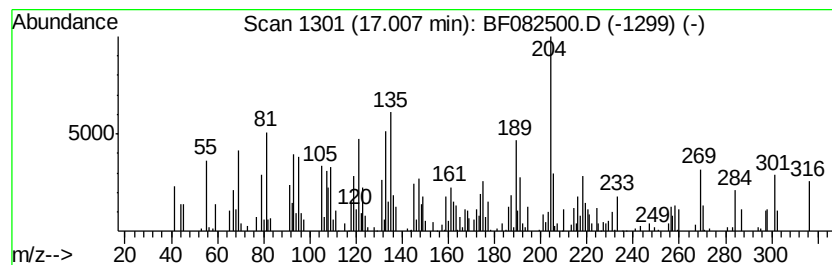
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 1,4-Dimethyl-8-isopropylide... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.01	4.25 ng	115125	Perylene-d12	15.50	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1000140-07-7	87
2	Selina-6-en-4-ol	222	C15H26O	1000140-23-2	52
3	Guaia-3,9-diene	204	C15H24	000489-83-8	47
4	1,2,4,8-Tetramethylbicyclo[6.3.0...	204	C15H24	137235-51-9	45
5	2,5,5,8a-Tetramethyl-6,7,8,8a-te...	204	C14H20O	124957-09-1	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102315\
Data File : BF082500.D
Acq On : 24 Oct 2015 8:41
Operator : UM/IZ
Sample : G4116-11
Misc :
ALS Vial : 29 Sample Multiplier: 1

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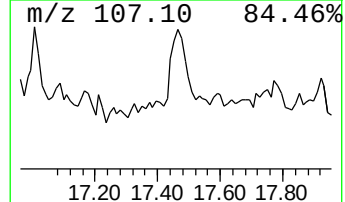
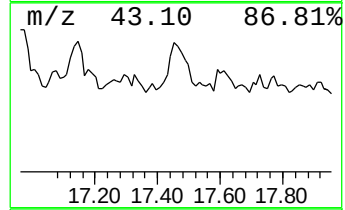
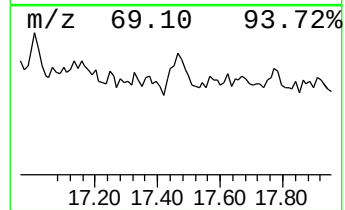
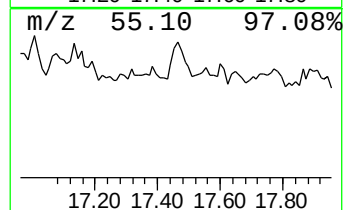
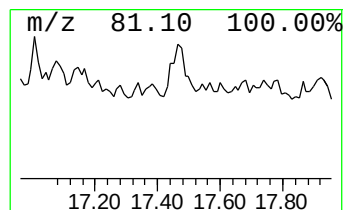
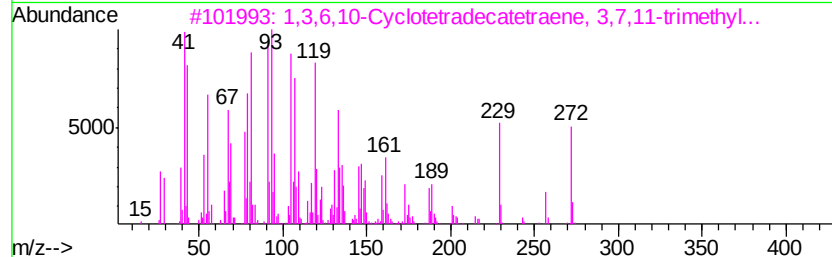
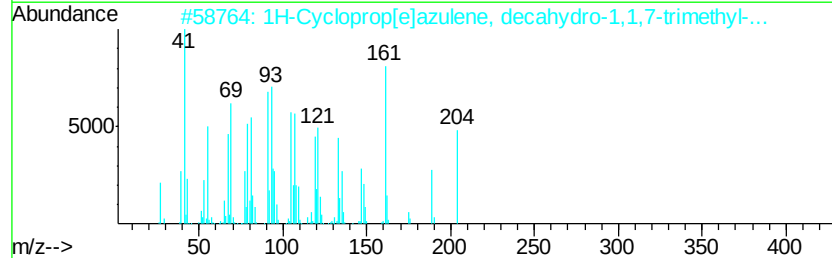
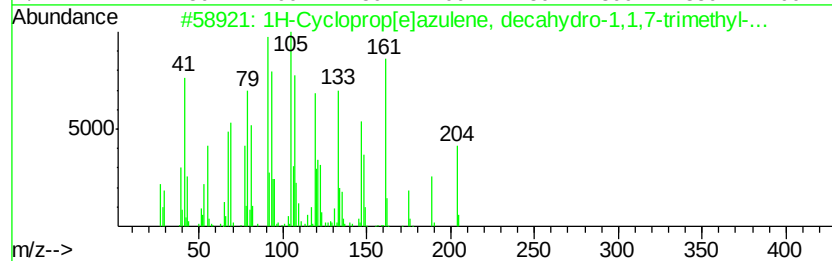
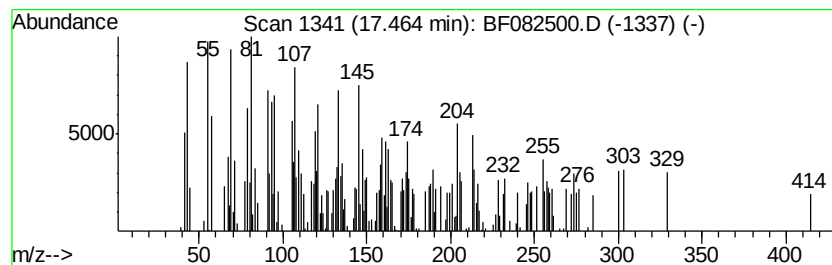
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown17.46 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.46	6.68 ng	180721	Perylene-d12	15.50

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Cycloprop[e]azulene, decahydr...	204	C15H24	025246-27-9	44
2			1H-Cycloprop[e]azulene, decahydr...	204	C15H24	072747-25-2	41
3			1,3,6,10-Cyclotetradecatetraene, ...	272	C20H32	001898-13-1	38
4			1H-Cycloprop[e]azulene, decahydr...	204	C15H24	000489-39-4	25
5			Naphthalene, decahydro-4a-methyl...	204	C15H24	017066-67-0	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102315\
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Acq On : 24 Oct 2015 8:41
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Sample : G4116-11
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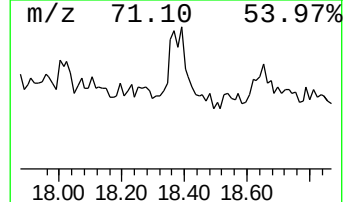
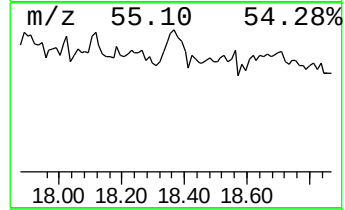
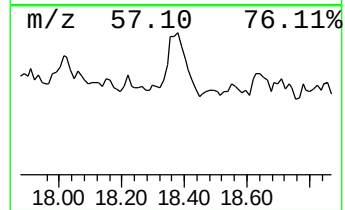
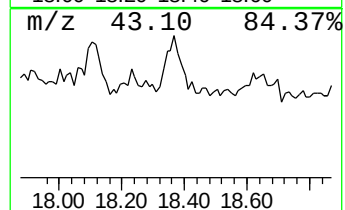
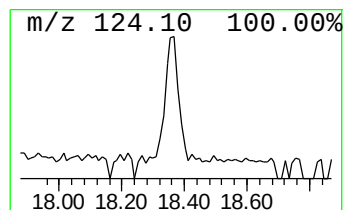
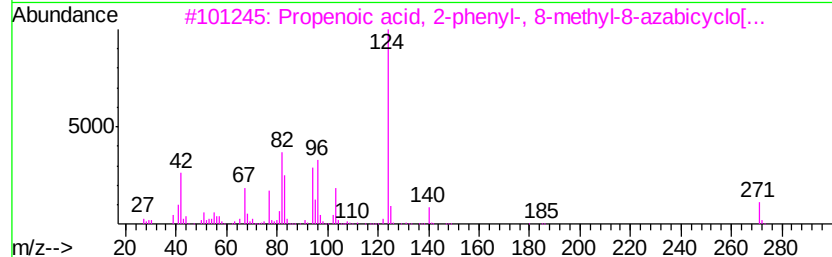
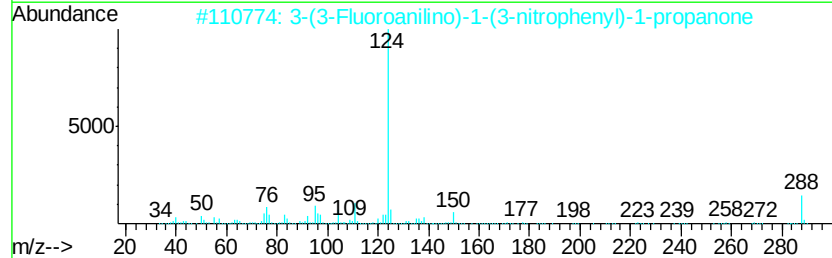
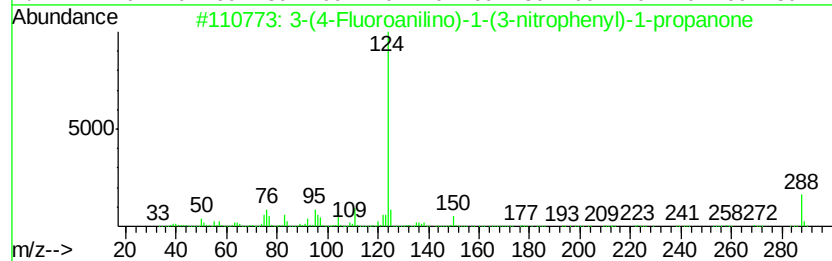
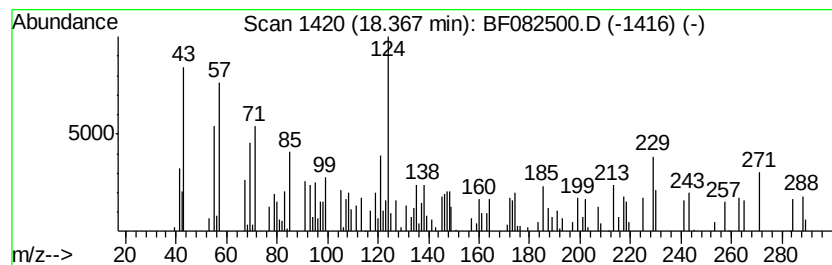
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BT-01(0-2)

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

Peak Number 15 unknown18.37 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
18.37	5.00 ng	135290	Perylene-d12	15.50		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-(4-Fluoroanilino)-1-(3-nitroph...	288	C15H13FN2O3	350039-84-8	25	
2	3-(3-Fluoroanilino)-1-(3-nitroph...	288	C15H13FN2O3	300726-64-1	25	
3	Propenoic acid, 2-phenyl-, 8-met...	271	C17H21NO2	1000289-44-7	22	
4	O-[n-Propylcarbamoyl]-6-cyanotro...	262	C13H18N4O2	1000211-90-2	14	
5	6-Methyl-2,4-pyrimidinediamine	124	C5H8N4	001791-73-7	14	



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102315\
Data File : BF082500.D
Acq On : 24 Oct 2015 8:41
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...	4.93	61.6	ng	1514820	1	6.75	491482	20.0
unknown6.53	6.53	97.8	ng	2403180	1	6.75	491482	20.0
Eicosane	10.70	2.6	ng	81627	4	11.29	618634	20.0
Undecanoic acid	11.82	3.7	ng	113550	4	11.29	618634	20.0
2-Chloropropioni...	14.55	4.4	ng	121823	5	13.98	549743	20.0
Oxirane, heptadecyl-	14.98	2.2	ng	58738	6	15.50	541272	20.0
Nonadecane	15.17	2.3	ng	62924	6	15.50	541272	20.0
1-Octadecanol	15.24	4.7	ng	126392	6	15.50	541272	20.0
Tridecane, 1-iodo-	15.94	2.6	ng	70502	6	15.50	541272	20.0
1,4-Dimethyl-8-is...	17.01	4.3	ng	115125	6	15.50	541272	20.0
unknown17.46	17.46	6.7	ng	180721	6	15.50	541272	20.0
unknown18.37	18.37	5.0	ng	135290	6	15.50	541272	20.0