

Data Path : Z:\HPCHEM1\BNA F\DATA\BF110815\
 Data File : BF082788.D
 Acq On : 7 Nov 2015 4:14
 Operator : UM/IZ
 Sample : G4257-03
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WABUT-2(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-BF110715.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.807	60	63	67	rVB	54948	88435	1.21%	0.123%
2	4.384	198	201	204	rVB	59801	88350	1.21%	0.123%
3	5.036	254	258	268	rVB	2394838	3484271	47.56%	4.843%
4	5.458	291	295	297	rBV	5426352	6754004	92.19%	9.388%
5	6.476	381	384	387	rBV	4748004	6553034	89.45%	9.109%
6	6.613	393	396	399	rBV	5916529	5959067	81.34%	8.283%
7	6.841	414	416	418	rBV	1393053	1504801	20.54%	2.092%
8	7.002	428	430	433	rVB	4626432	4480953	61.17%	6.229%
9	7.413	462	466	468	rBV	3351085	4568643	62.36%	6.350%
10	8.133	526	529	531	rBV	2290650	2110847	28.81%	2.934%
11	9.207	620	623	626	rVV	5203357	7325798	100.00%	10.183%
12	9.607	655	658	660	rBV	1991641	2013287	27.48%	2.798%
13	9.802	672	675	676	rBV	84758	121761	1.66%	0.169%
14	9.836	676	678	680	rVV	200417	186160	2.54%	0.259%
15	9.882	680	682	684	rVV	1956973	2375389	32.42%	3.302%
16	10.019	692	694	695	rBV	82816	80363	1.10%	0.112%
17	10.305	717	719	720	rBV	165898	144928	1.98%	0.201%
18	10.328	720	721	723	rVB	139967	127603	1.74%	0.177%
19	10.545	738	740	743	rBV	56898	107829	1.47%	0.150%
20	10.670	748	751	754	rVV	4293267	4882395	66.65%	6.787%
21	10.716	754	755	757	rVV	117052	121458	1.66%	0.169%
22	10.808	761	763	769	rVB2	216346	364593	4.98%	0.507%
23	11.253	799	802	803	rBV	310578	278559	3.80%	0.387%
24	11.288	803	805	807	rVB	57644	77619	1.06%	0.108%
25	11.368	809	812	814	rVV	2930569	2517278	34.36%	3.499%
26	11.436	814	818	820	rVB2	49987	89748	1.23%	0.125%
27	11.676	837	839	842	rBV	178236	163926	2.24%	0.228%
28	11.905	857	859	863	rBV2	193138	259059	3.54%	0.360%
29	12.088	871	875	879	rVB2	54457	117826	1.61%	0.164%
30	12.694	926	928	934	rBV3	44981	81383	1.11%	0.113%
31	12.785	934	936	939	rVV2	455213	515167	7.03%	0.716%
32	12.865	939	943	945	rVV2	88509	99905	1.36%	0.139%
33	12.956	948	951	954	rBV	6289721	7079074	96.63%	9.840%
34	13.071	958	961	963	rVB	91779	118759	1.62%	0.165%

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

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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.288	974	980	984	rVB4	38696	93579	1.28%	0.130%
36	13.391	987	989	992	rBV	721123	805504	11.00%	1.120%
37	13.494	996	998	1001	rVV	457918	393491	5.37%	0.547%
38	13.882	1029	1032	1040	rBV3	261168	946839	12.92%	1.316%
39	13.996	1040	1042	1045	rVB	1958795	2311219	31.55%	3.213%
40	14.191	1056	1059	1061	rVB	72302	84259	1.15%	0.117%
41	14.488	1083	1085	1087	rBV	78075	82926	1.13%	0.115%
42	14.568	1087	1092	1097	rBV7	26231	110170	1.50%	0.153%
43	14.865	1116	1118	1120	rVB	153908	148867	2.03%	0.207%
44	15.117	1138	1140	1143	rBV	83388	92835	1.27%	0.129%
45	15.425	1164	1167	1170	rBV	1539818	1837815	25.09%	2.555%
46	15.894	1206	1208	1211	rBV	54676	90050	1.23%	0.125%
47	17.471	1341	1346	1351	rBV9	23480	101959	1.39%	0.142%

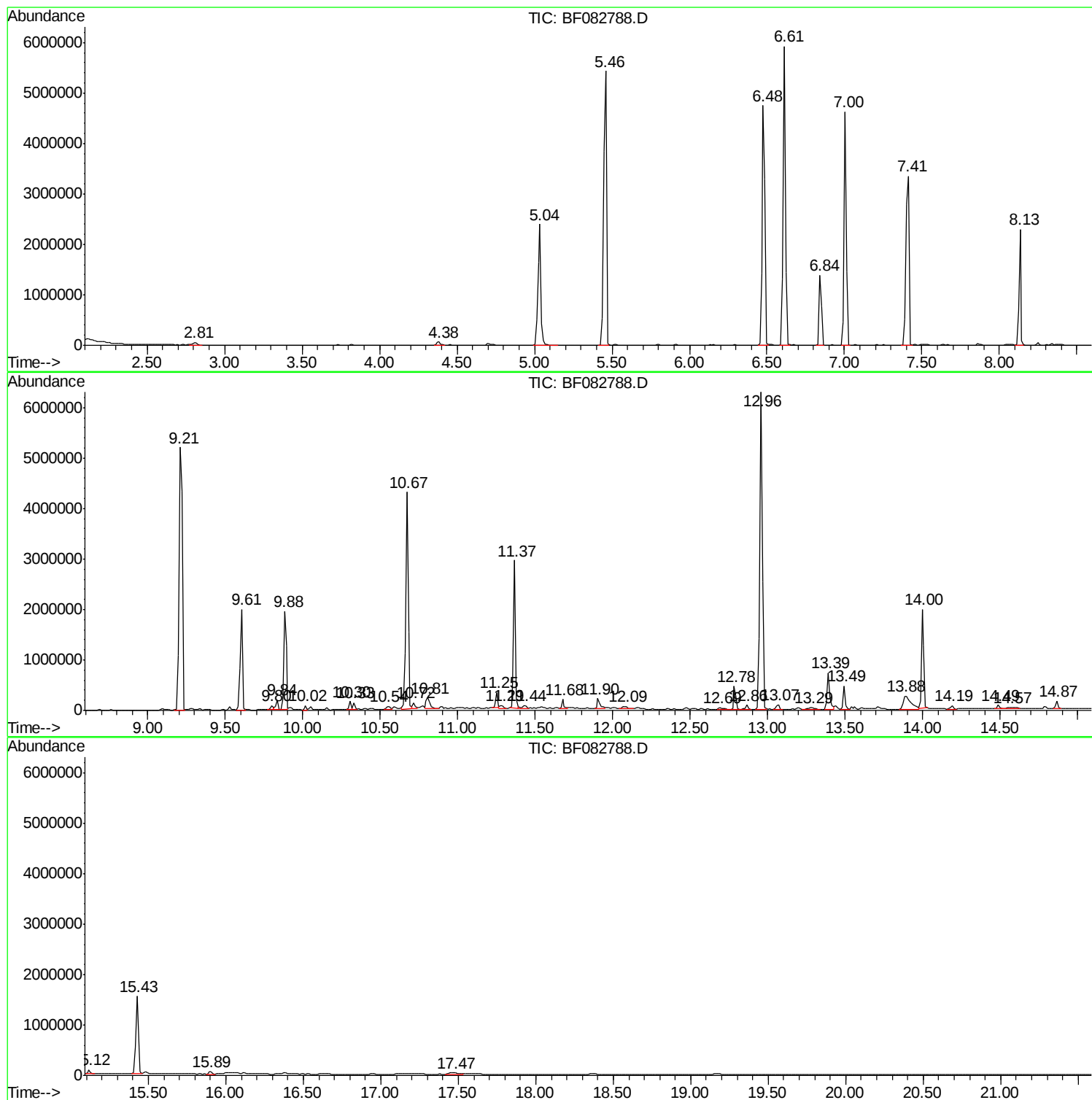
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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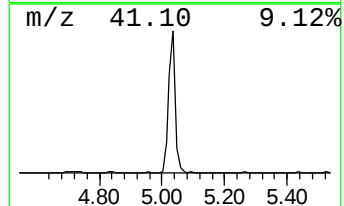
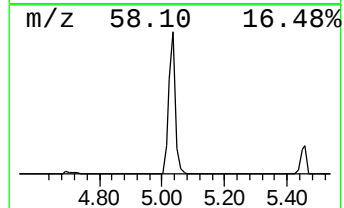
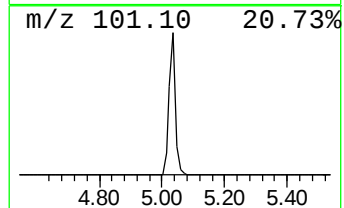
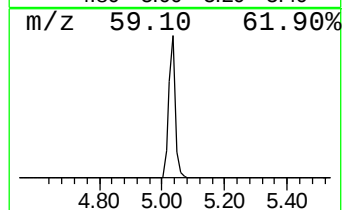
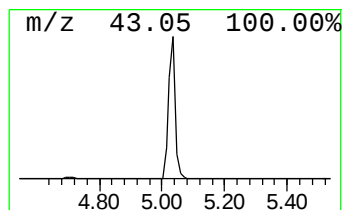
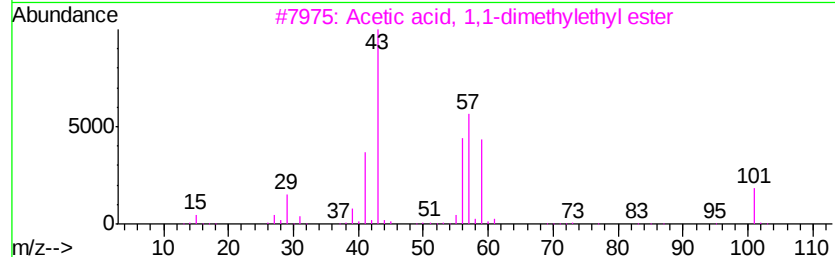
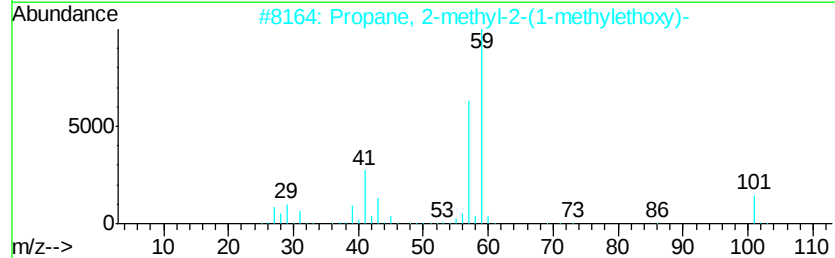
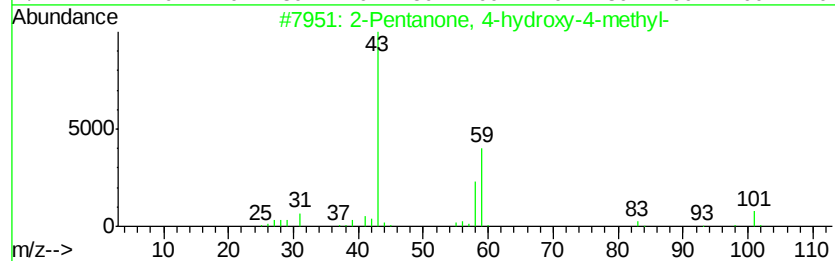
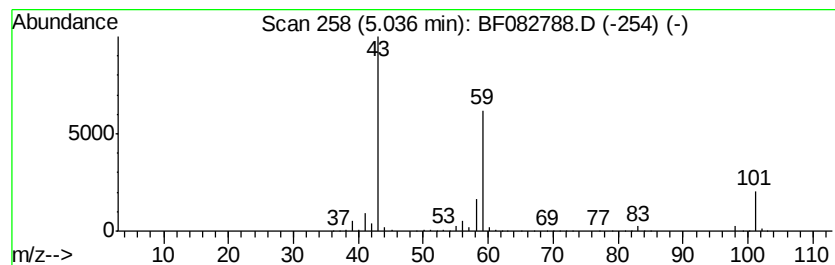
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	46.31 ng	3484270	1,4-Dichlorobenzene-d4	6.84

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	53
3		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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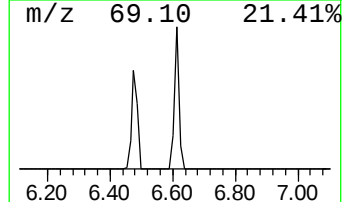
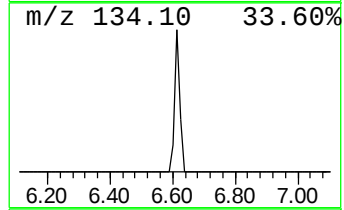
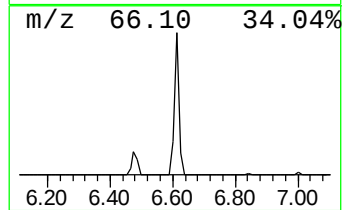
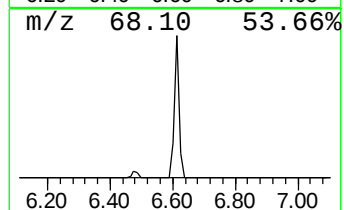
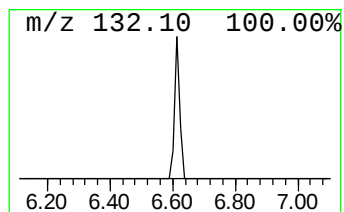
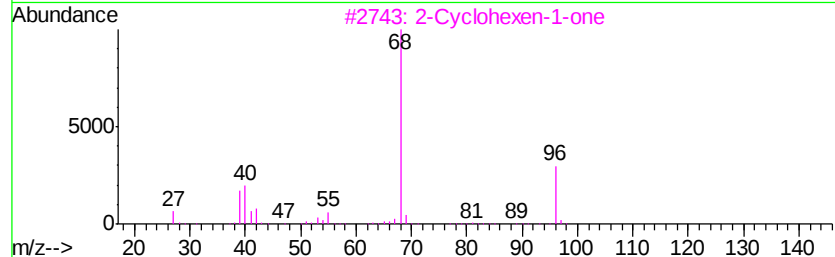
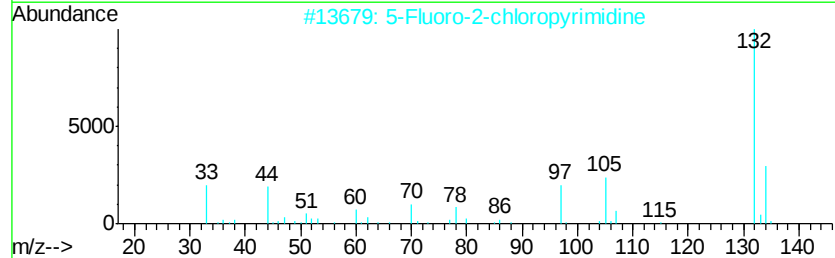
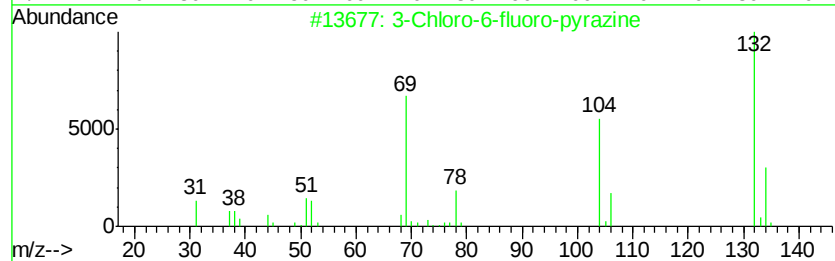
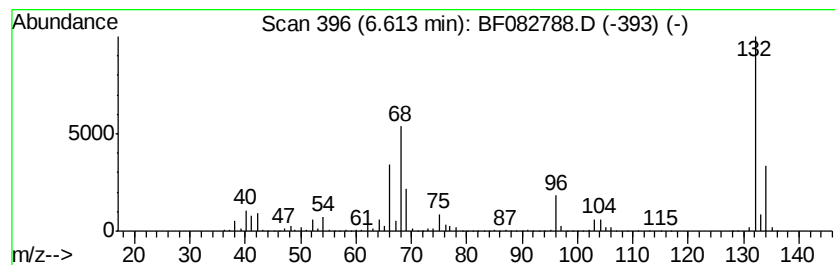
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	79.20 ng	5959070	1,4-Dichlorobenzene-d4	6.84

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		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
4		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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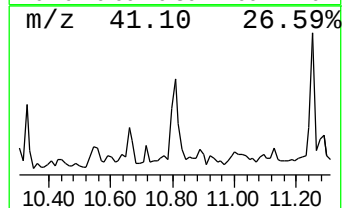
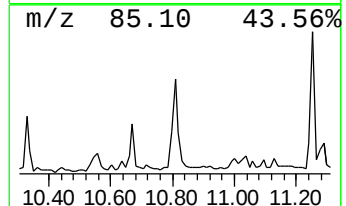
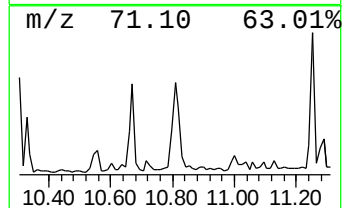
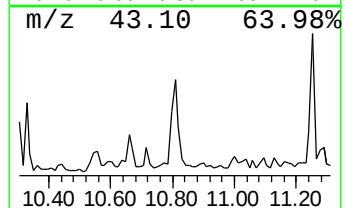
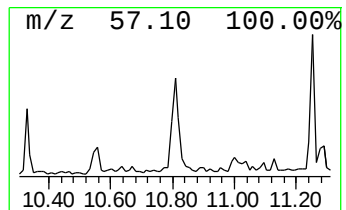
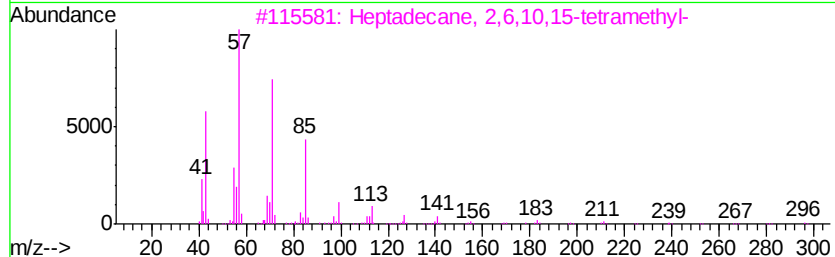
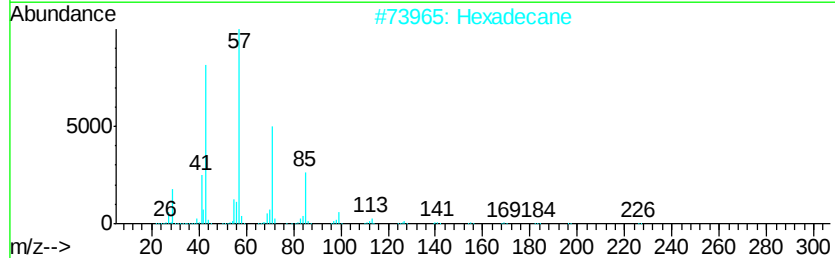
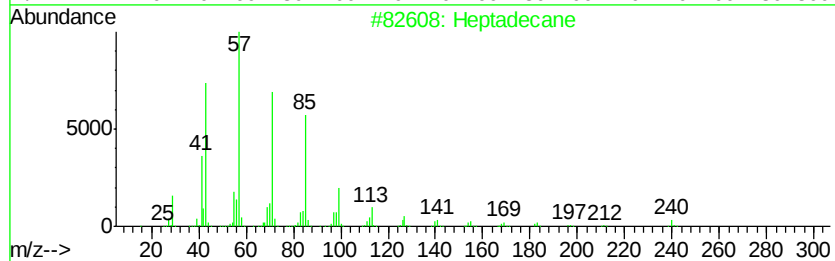
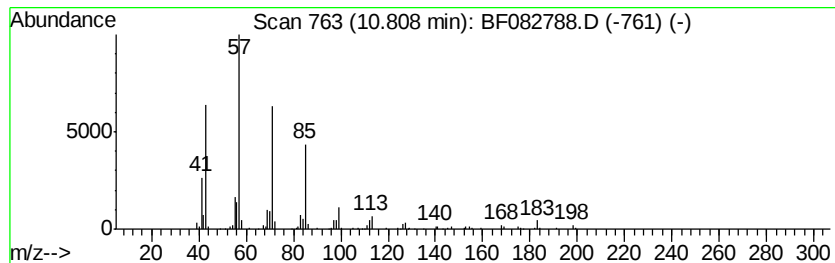
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Heptadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.81	2.90 ng	364593	Phenanthrene-d10	11.37

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	90
2	Hexadecane		226	C16H34	000544-76-3	90
3	Heptadecane, 2,6,10,15-tetramethyl-		296	C21H44	054833-48-6	86
4	Pentadecane		212	C15H32	000629-62-9	86
5	Octadecane		254	C18H38	000593-45-3	83



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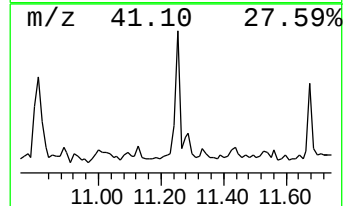
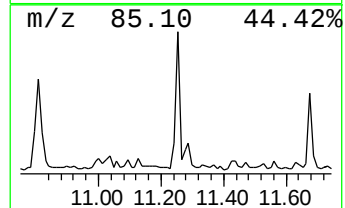
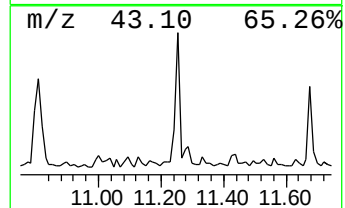
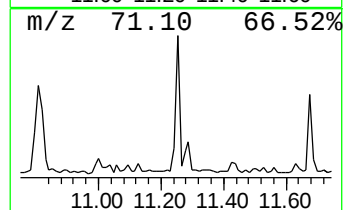
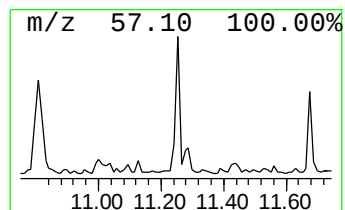
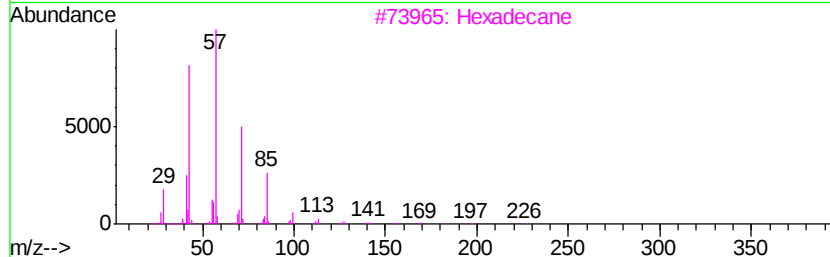
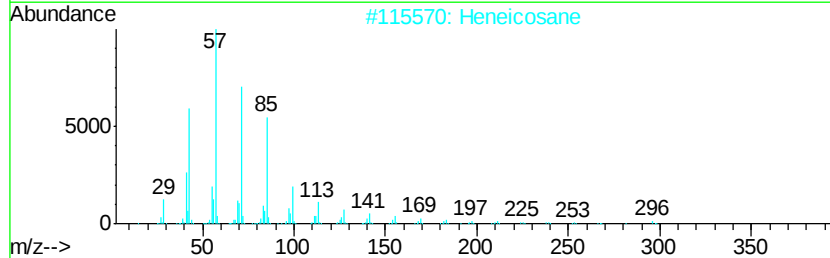
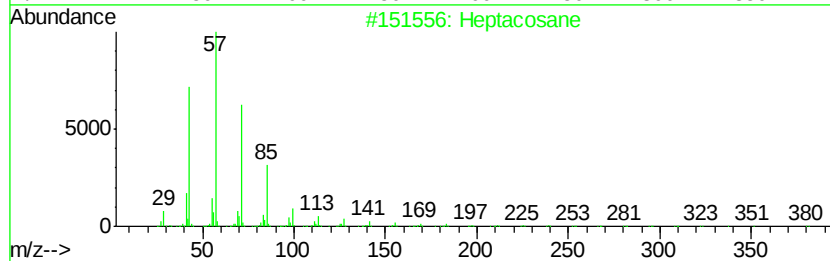
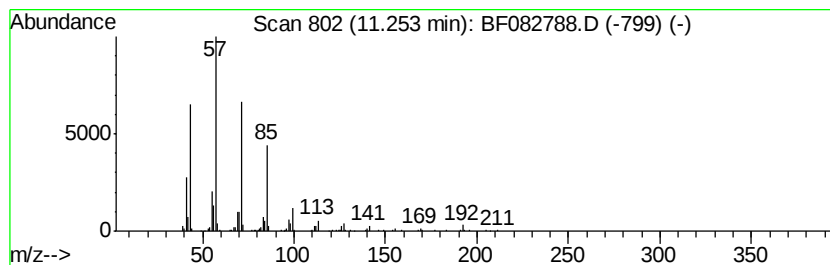
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.25	2.21 ng	278559	Phenanthrene-d10	11.37

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	91
2	Heneicosane		296	C21H44	000629-94-7	90
3	Hexadecane		226	C16H34	000544-76-3	90
4	Dodecane, 2-methyl-6-propyl-		226	C16H34	055045-08-4	86
5	Heptadecane, 8-methyl-		254	C18H38	013287-23-5	80



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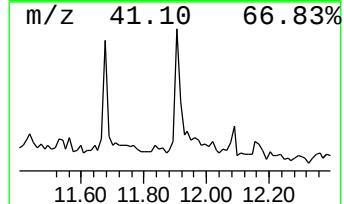
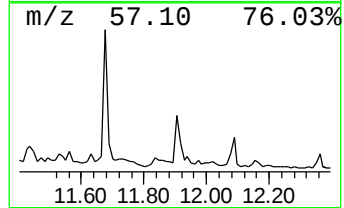
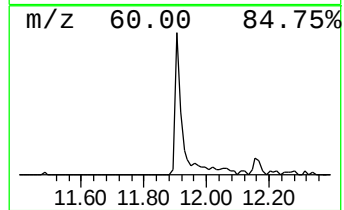
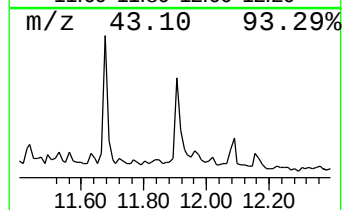
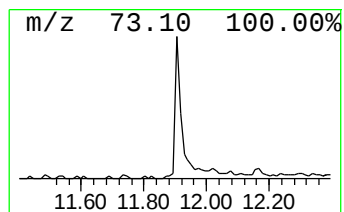
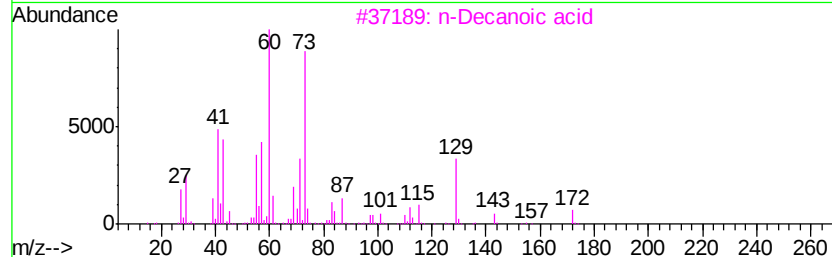
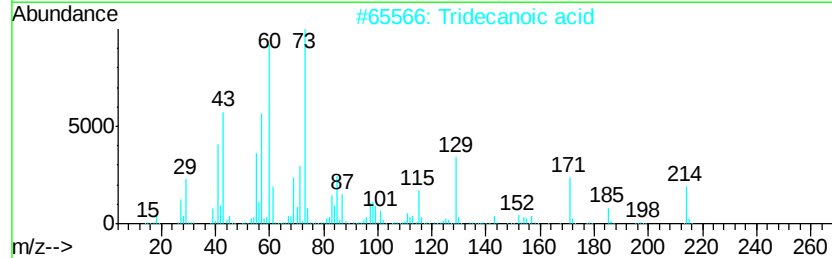
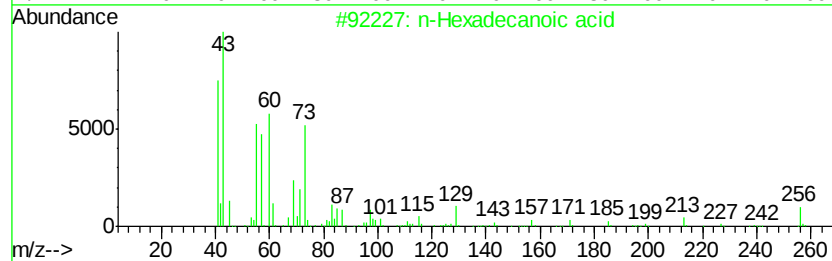
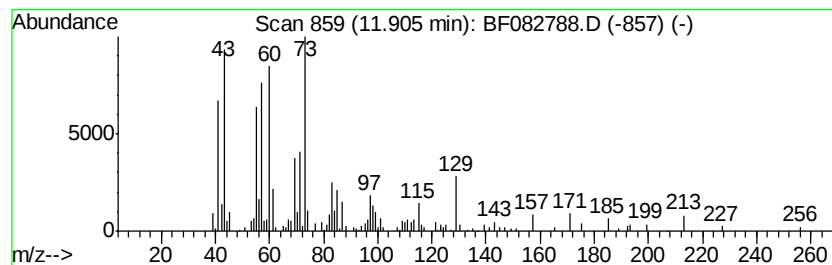
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	2.06 ng	259059	Phenanthrene-d10	11.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2		Tridecanoic acid	214	C13H26O2	000638-53-9	86
3		n-Decanoic acid	172	C10H20O2	000334-48-5	72
4		Undecanoic acid	186	C11H22O2	000112-37-8	72
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	64



Data Path : Z:\HPCHEM1\BNA F\DATA\BF110815\
Data File : BF082788.D
Acq On : 7 Nov 2015 4:14
Operator : UM/IZ
Sample : G4257-03
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WABUT-2(0-2)

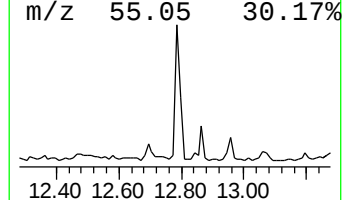
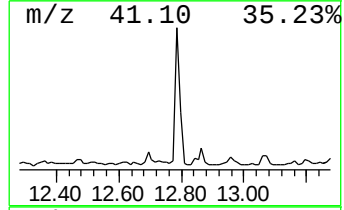
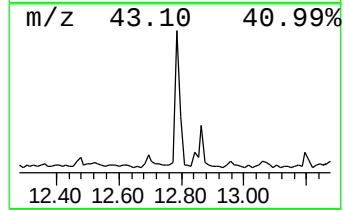
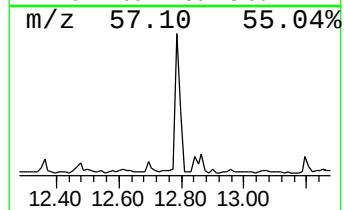
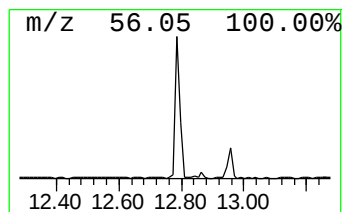
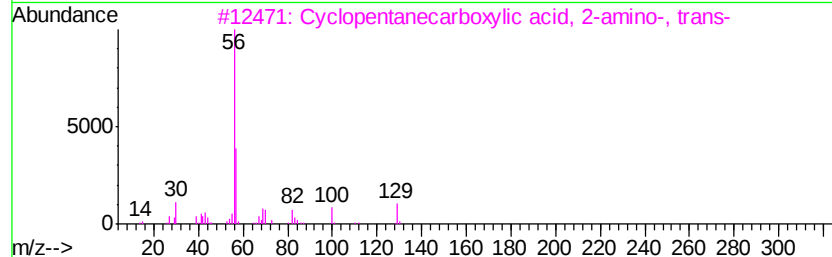
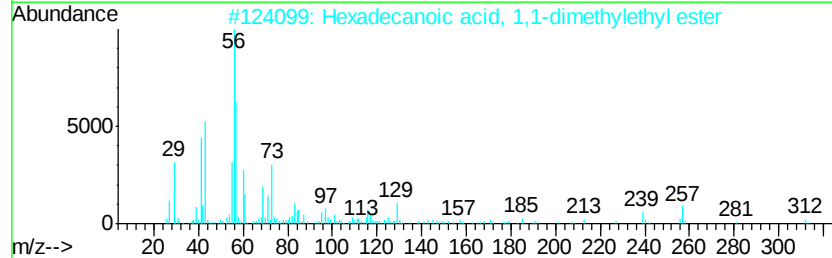
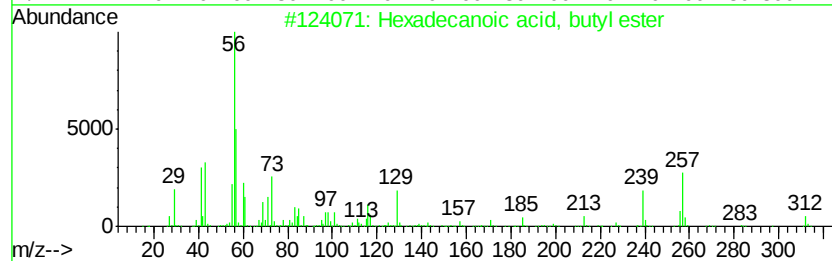
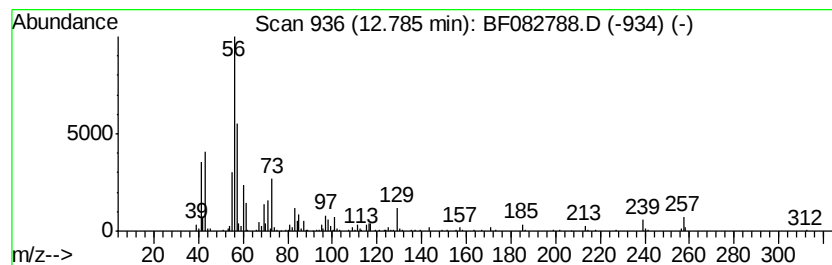
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.78	4.46 ng	515167	Chrysene-d12	14.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	93
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	53
3		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	46
4		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	43
5		2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	40



Data Path : Z:\HPCHEM1\BNA F\DATA\BF110815\
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Acq On : 7 Nov 2015 4:14
Operator : UM/IZ
Sample : G4257-03
Misc :
ALS Vial : 26 Sample Multiplier: 1

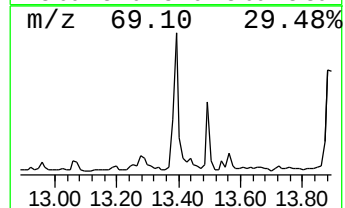
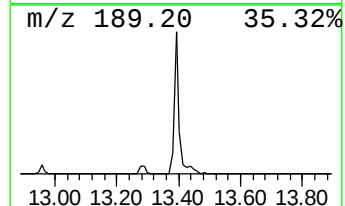
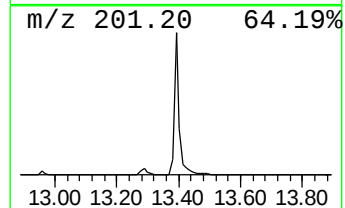
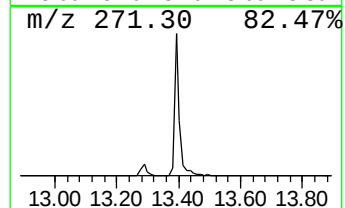
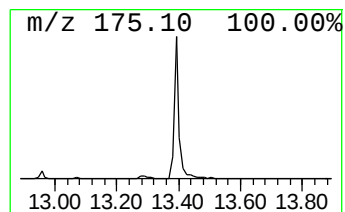
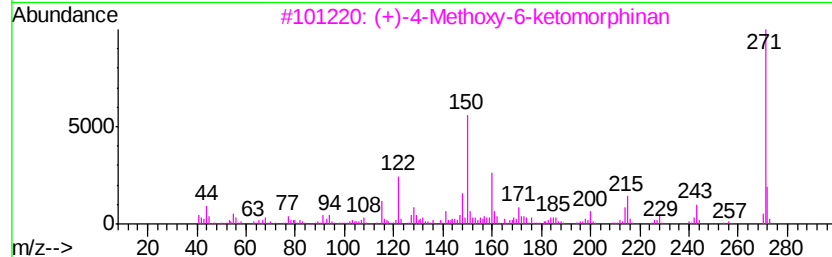
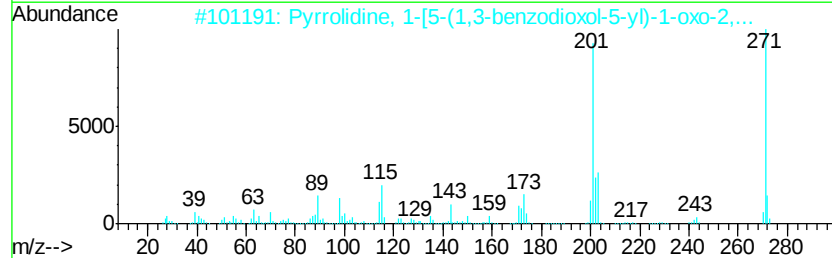
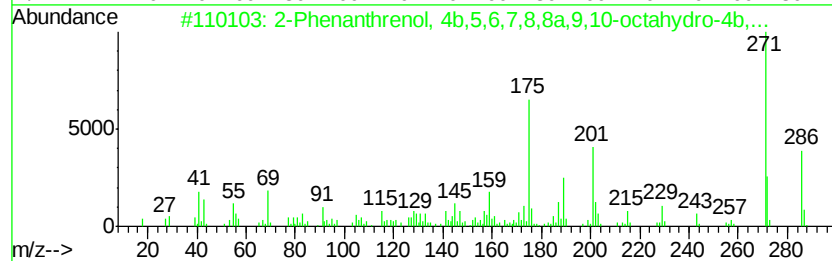
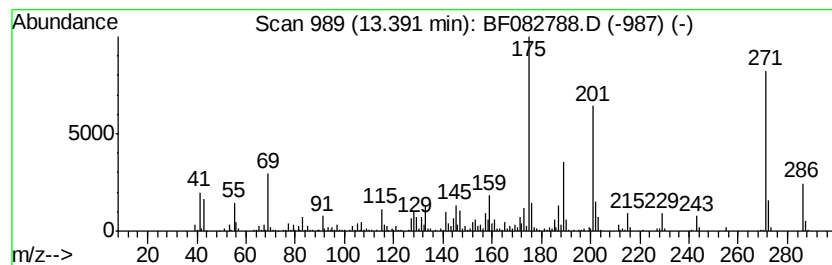
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.39	6.97 ng	805504	Chrysene-d12	14.00	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	96
2	Pyrrolidine, 1-[5-(1,3-benzodiox...	271	C16H17NO3	025924-78-1	43
3	(+)-4-Methoxy-6-ketomorphinan	271	C17H21NO2	1000129-08-5	22
4	Desomorphine	271	C17H21NO2	000427-00-9	22
5	1-Methyl-3-phenyl-4-azafluorenone	271	C19H13NO	069751-55-9	22



Data Path : Z:\HPCHEM1\BNA F\DATA\BF110815\
Data File : BF082788.D
Acq On : 7 Nov 2015 4:14
Operator : UM/IZ
Sample : G4257-03
Misc :
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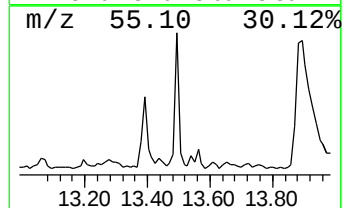
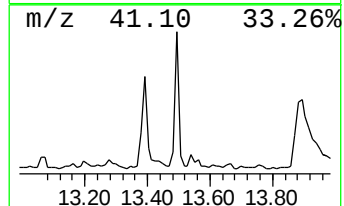
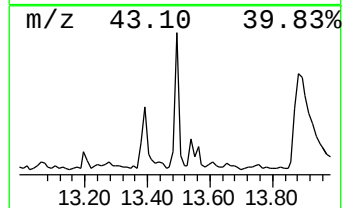
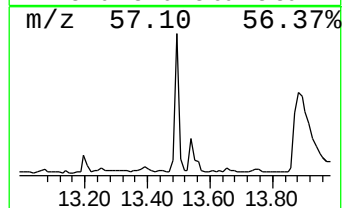
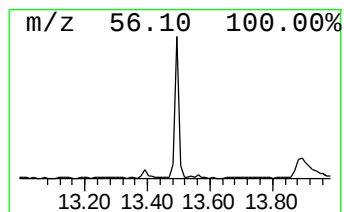
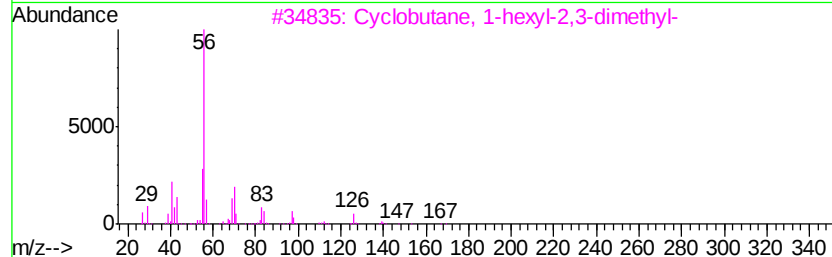
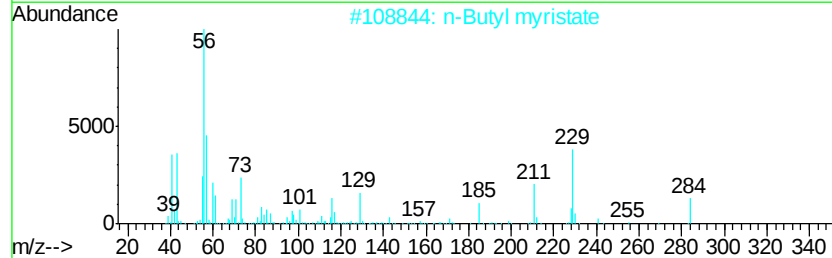
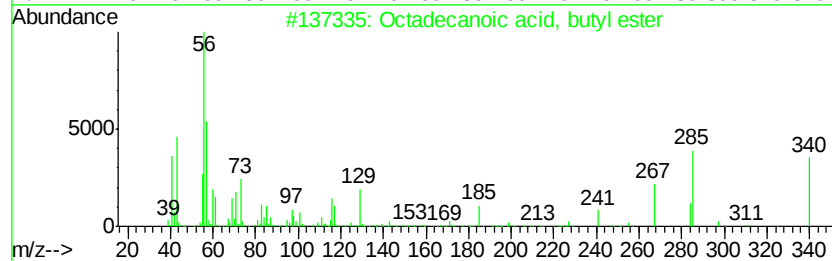
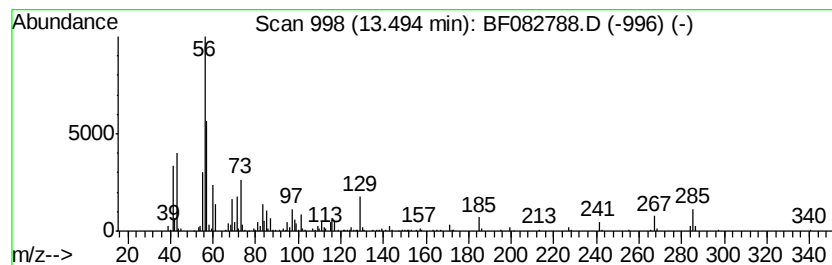
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.49	3.41 ng	393491	Chrysene-d12		14.00
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	94
2	n-Butyl myristate	284	C18H36O2	000110-36-1	86
3	Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	38
4	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	38
5	Pentadecane, 8-methylene-	224	C16H32	055668-09-2	37



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110815\
Data File : BF082788.D
Acq On : 7 Nov 2015 4:14
Operator : UM/IZ
Sample : G4257-03
Misc :
ALS Vial : 26 Sample Multiplier: 1

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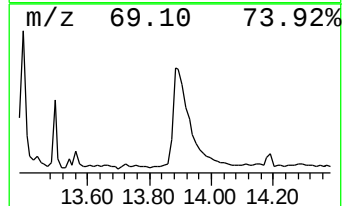
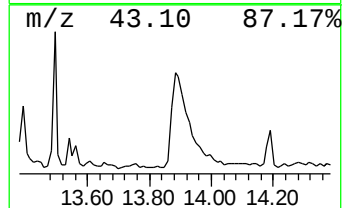
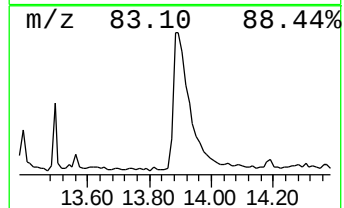
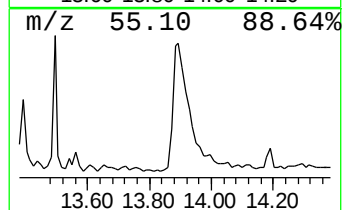
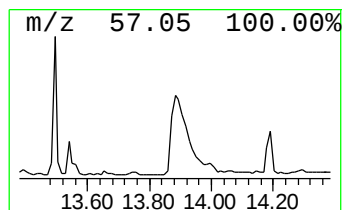
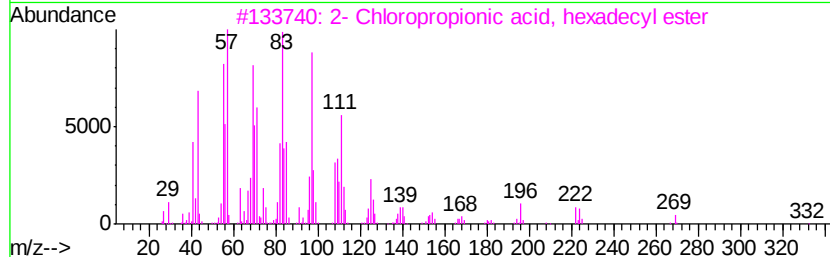
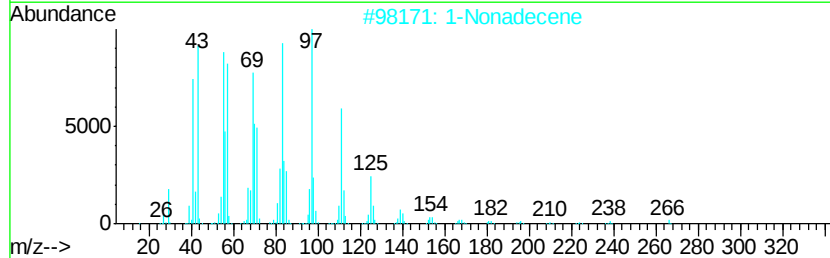
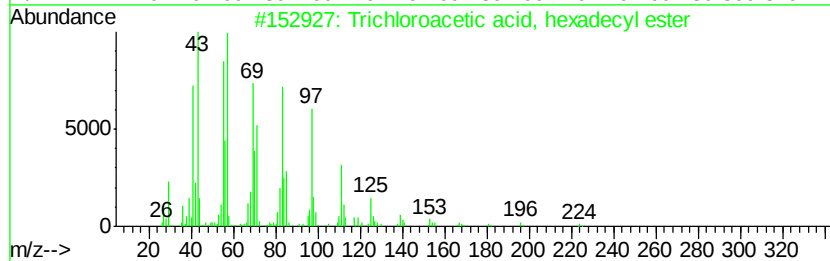
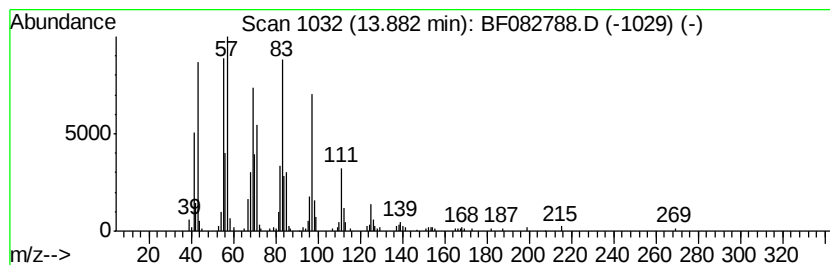
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Trichloroacetic acid, hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	8.19 ng	946839	Chrysene-d12	14.00

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
2			1-Nonadecene	266	C19H38	018435-45-5	91
3			2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	91
4			Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
5			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110815\
Data File : BF082788.D
Acq On : 7 Nov 2015 4:14
Operator : UM/IZ
Sample : G4257-03
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WABUT-2(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.04	46.3	ng	3484270	1	6.84	1504800	20.0
unknown6.61	6.61	79.2	ng	5959070	1	6.84	1504800	20.0
Heptadecane	10.81	2.9	ng	364593	4	11.37	2517280	20.0
Heptacosane	11.25	2.2	ng	278559	4	11.37	2517280	20.0
n-Hexadecanoic acid	11.90	2.1	ng	259059	4	11.37	2517280	20.0
Hexadecanoic acid...	12.78	4.5	ng	515167	5	14.00	2311220	20.0
2-Phenanthrenol, ...	13.39	7.0	ng	805504	5	14.00	2311220	20.0
Octadecanoic acid...	13.49	3.4	ng	393491	5	14.00	2311220	20.0
Trichloroacetic a...	13.88	8.2	ng	946839	5	14.00	2311220	20.0