

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110815\
 Data File : BF082789.D
 Acq On : 7 Nov 2015 4:43
 Operator : UM/IZ
 Sample : G4257-05
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WABUT-3(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	5.036	254	258	265	rBV	2367918	3478775	47.70%	5.035%
2	5.459	291	295	297	rBV	5372524	6700654	91.88%	9.699%
3	6.476	381	384	387	rBV	4711905	6594582	90.42%	9.545%
4	6.613	393	396	399	rBV	5900625	6001336	82.29%	8.687%
5	6.842	414	416	418	rBV	1346967	1526423	20.93%	2.209%
6	7.002	428	430	433	rBV	4708318	4629076	63.47%	6.700%
7	7.413	462	466	468	rBV	3374440	4558686	62.51%	6.598%
8	8.133	526	529	531	rBV	2287782	2129190	29.20%	3.082%
9	9.208	620	623	626	rBV	5277468	7292947	100.00%	10.556%
10	9.608	655	658	660	rBV	1582307	1665332	22.83%	2.410%
11	9.882	680	682	685	rVB	2065789	2361054	32.37%	3.418%
12	10.305	717	719	720	rBV	194924	165835	2.27%	0.240%
13	10.328	720	721	723	rVB	113781	101793	1.40%	0.147%
14	10.556	737	741	743	rBV	45878	76576	1.05%	0.111%
15	10.671	748	751	754	rBV	4346121	4620356	63.35%	6.688%
16	10.808	761	763	767	rVB	151879	253870	3.48%	0.367%
17	11.254	800	802	803	rBV	232669	212926	2.92%	0.308%
18	11.368	809	812	814	rBV	2915056	2530531	34.70%	3.663%
19	11.437	814	818	822	rVB3	42401	78481	1.08%	0.114%
20	11.677	837	839	842	rVB	150054	127749	1.75%	0.185%
21	11.905	857	859	864	rBV2	233396	345648	4.74%	0.500%
22	12.785	934	936	939	rVB	361056	346662	4.75%	0.502%
23	12.865	939	943	945	rVB2	75710	87007	1.19%	0.126%
24	12.957	948	951	954	rBV	6996031	6914423	94.81%	10.008%
25	13.494	996	998	1000	rBV	329381	277640	3.81%	0.402%
26	13.882	1029	1032	1040	rBV	397262	1148392	15.75%	1.662%
27	13.997	1040	1042	1045	rVB	2052548	2285561	31.34%	3.308%
28	14.557	1087	1091	1095	rBV5	22873	78111	1.07%	0.113%
29	14.865	1115	1118	1120	rBV	174280	178744	2.45%	0.259%
30	15.117	1137	1140	1143	rBV	67525	81124	1.11%	0.117%
31	15.425	1164	1167	1170	rBV	1540229	1836025	25.18%	2.658%
32	15.894	1205	1208	1212	rBV	44962	76230	1.05%	0.110%
33	16.008	1213	1218	1226	rBV8	50843	228366	3.13%	0.331%
34	16.386	1243	1251	1256	rBV3	29697	96754	1.33%	0.140%

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Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WABUT-3(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

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

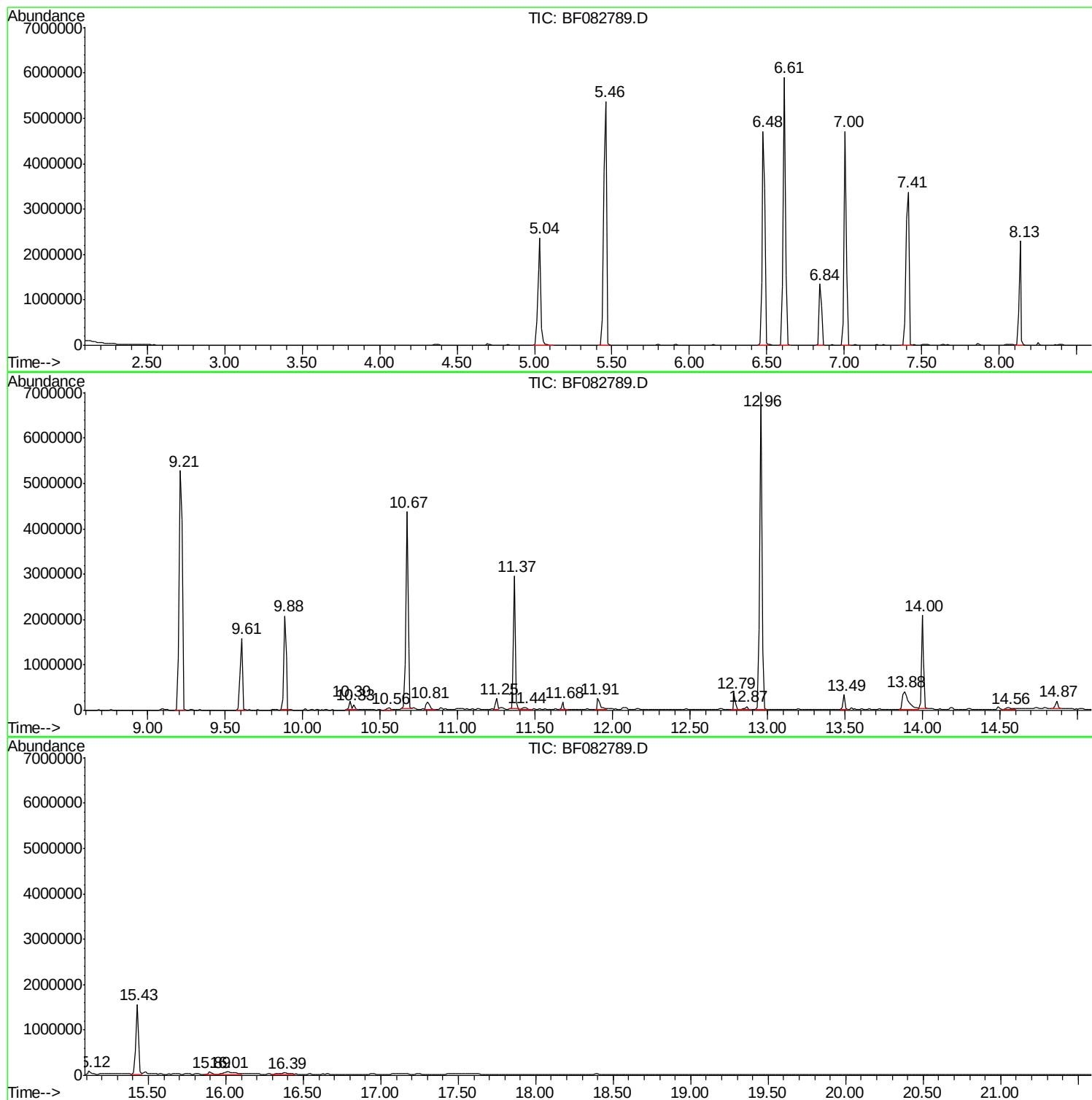
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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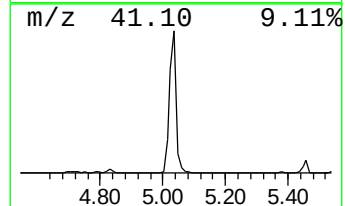
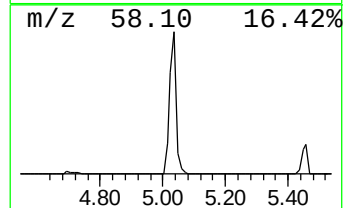
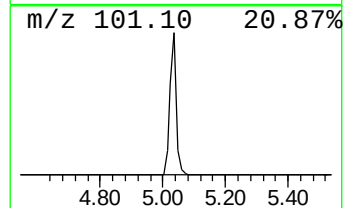
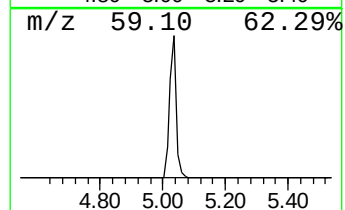
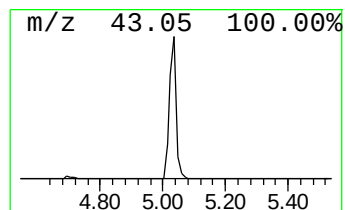
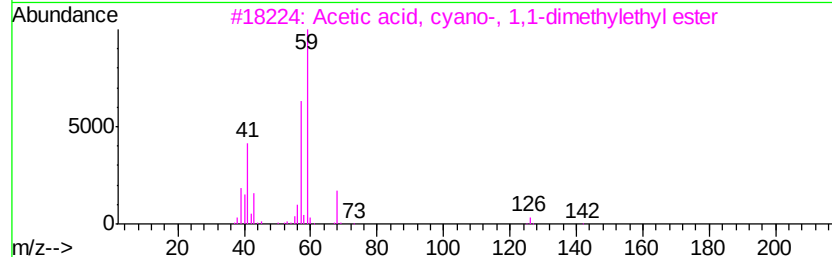
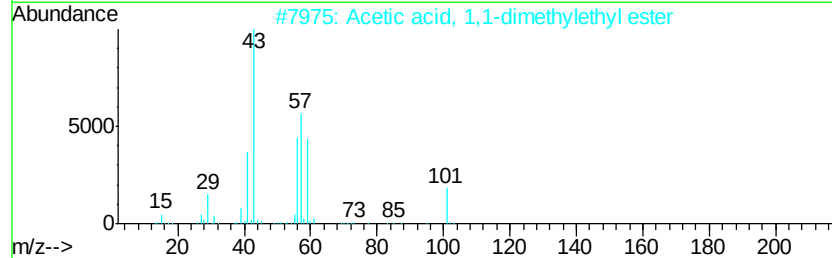
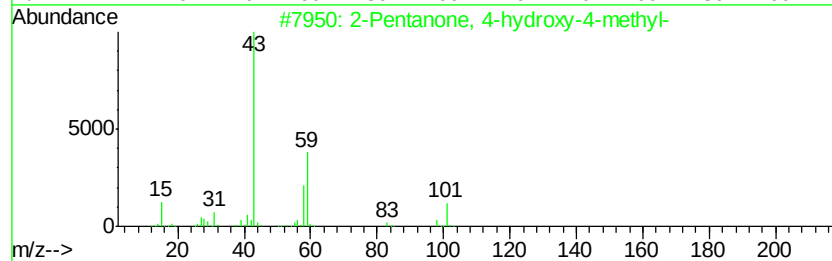
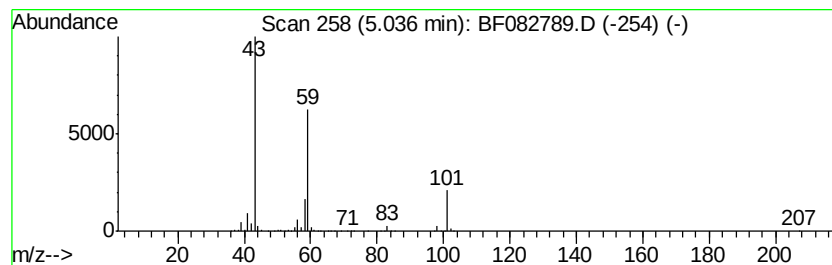
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	45.58 ng	3478780	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	72
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9



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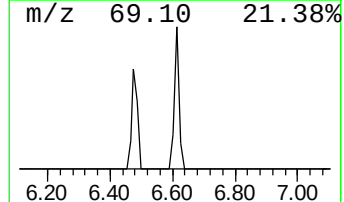
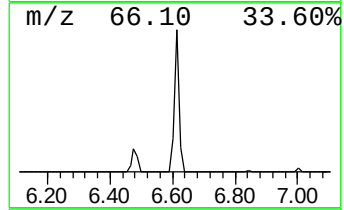
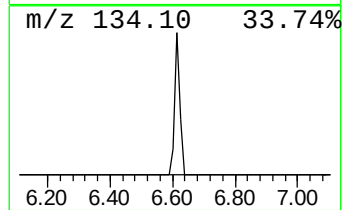
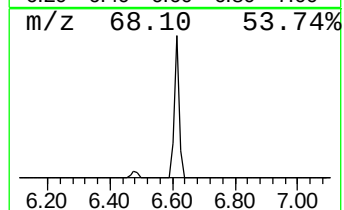
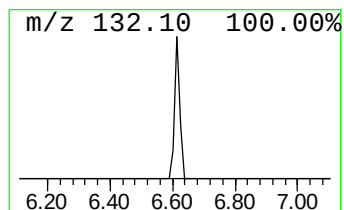
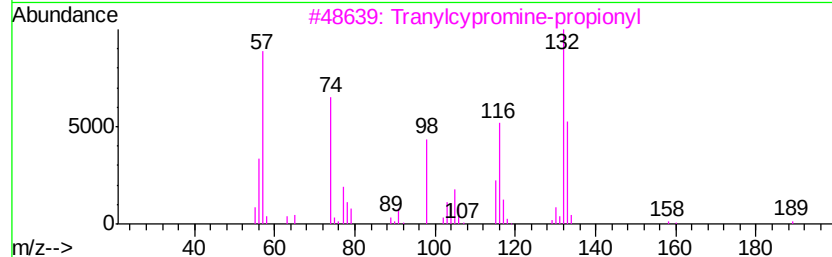
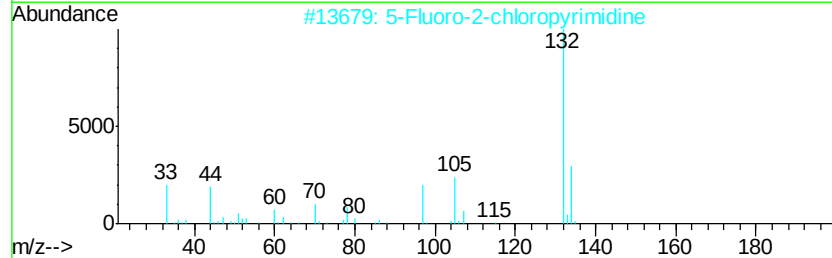
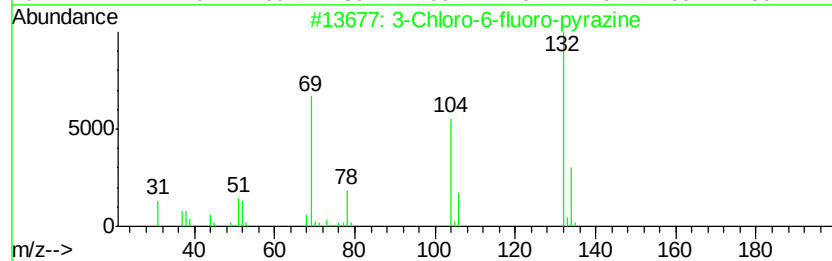
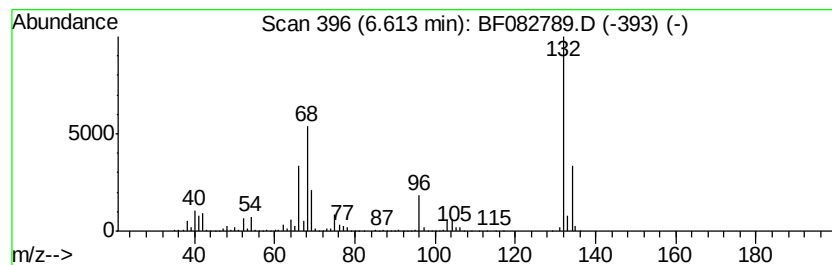
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	78.63 ng	6001340	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		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
5		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10



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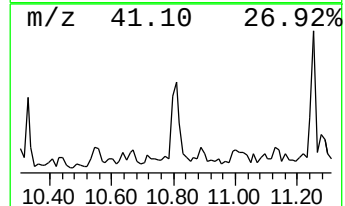
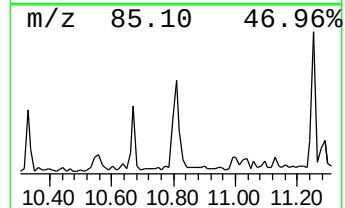
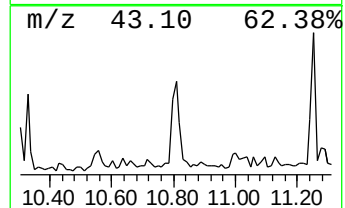
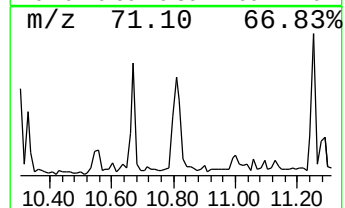
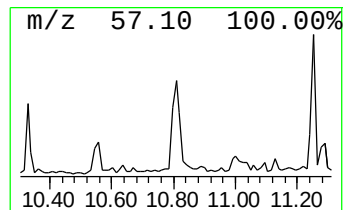
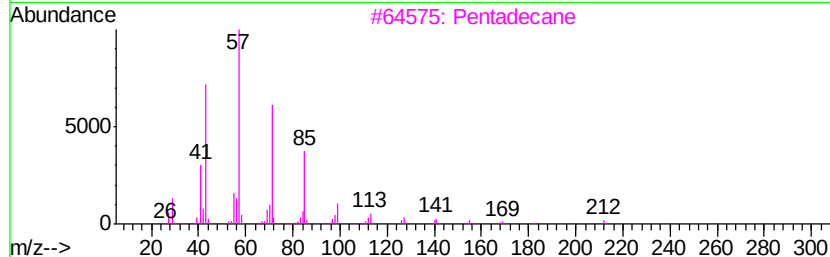
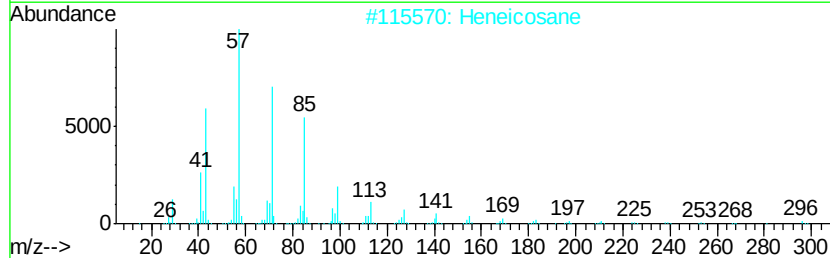
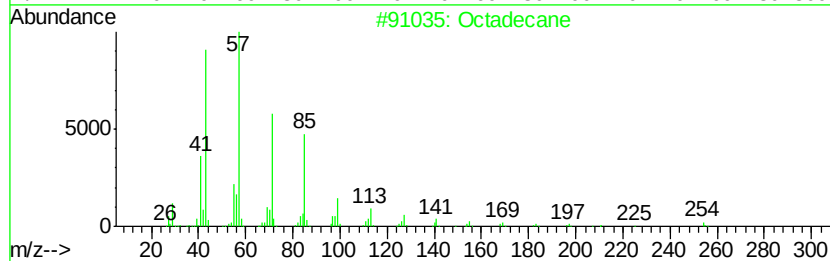
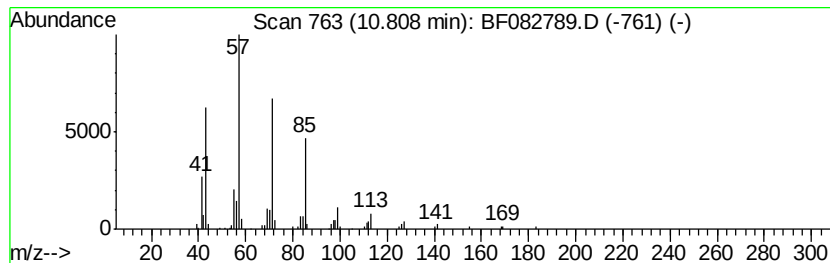
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.81	2.01 ng	253870	Phenanthrene-d10	11.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane	254	C18H38	000593-45-3	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Pentadecane	212	C15H32	000629-62-9	90
4		Hexadecane	226	C16H34	000544-76-3	90
5		Nonadecane	268	C19H40	000629-92-5	87



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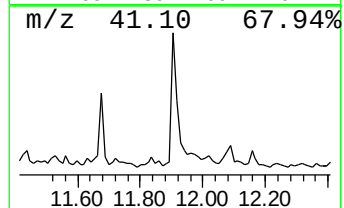
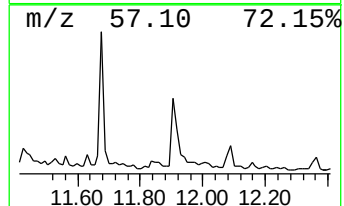
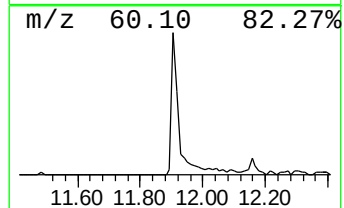
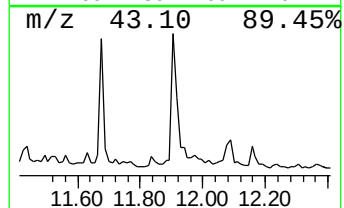
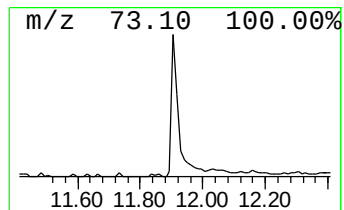
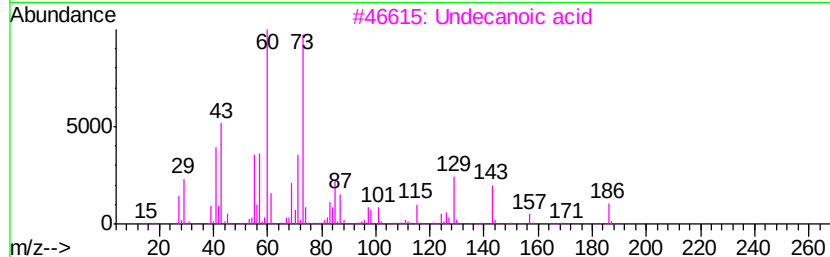
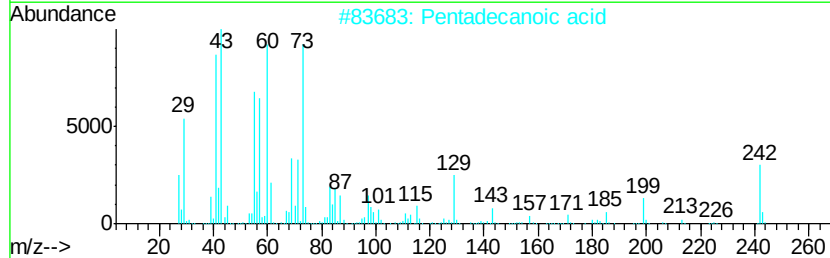
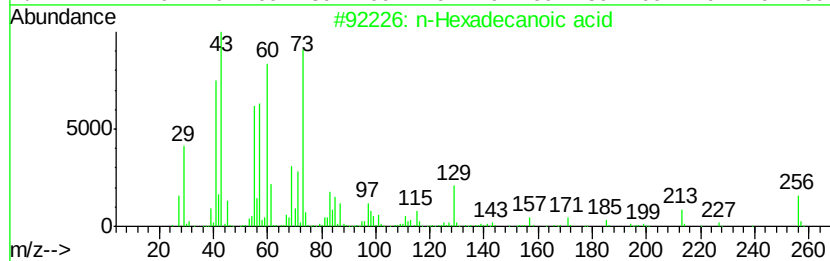
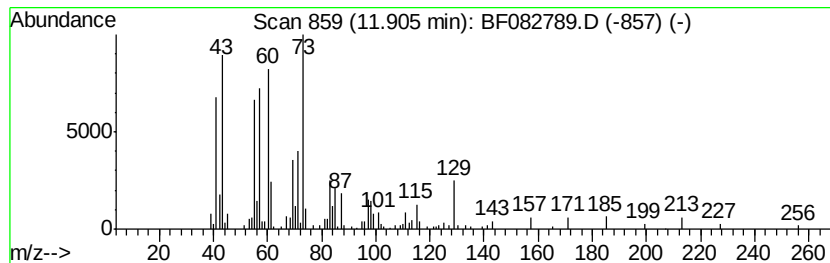
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.91	2.73 ng	345648	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Undecanoic acid	186	C11H22O2	000112-37-8	86
4	Tridecanoic acid	214	C13H26O2	000638-53-9	86
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	78



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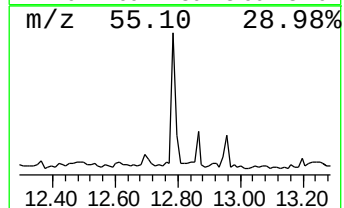
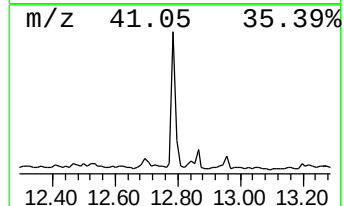
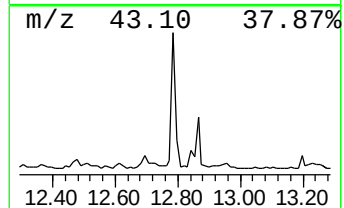
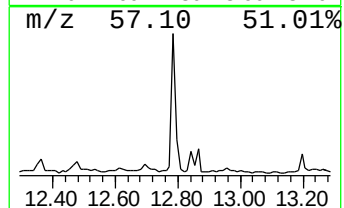
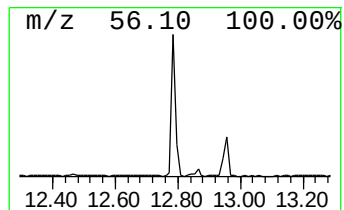
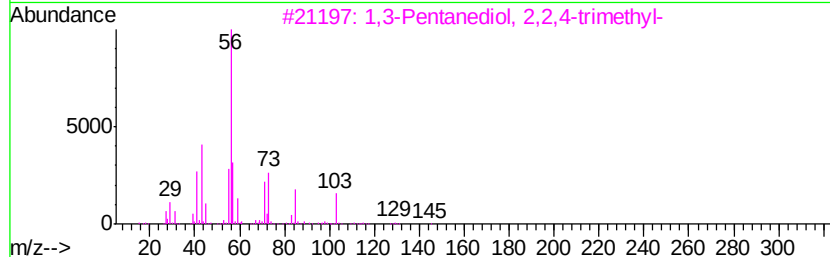
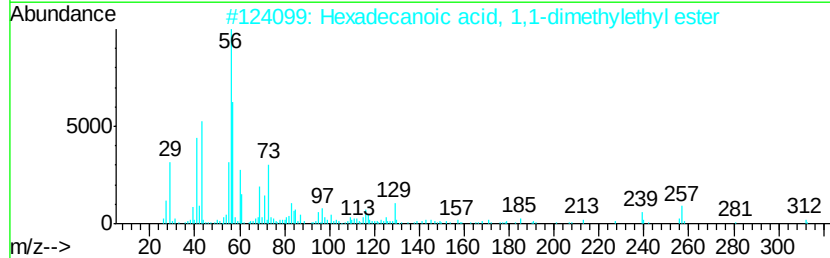
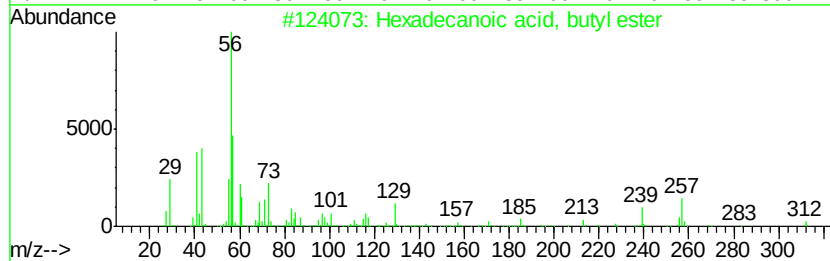
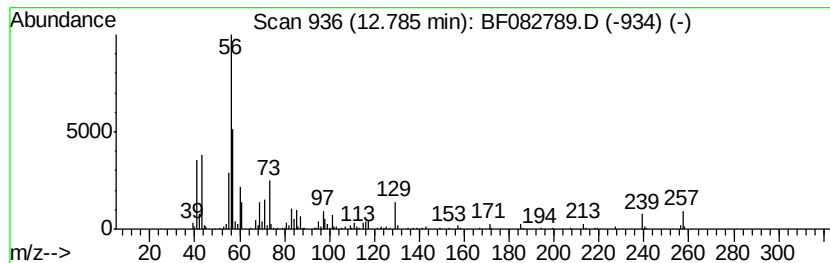
Instrument :
BNA_F
ClientSampleId :
WABUT-3(0-2)

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

Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.79	3.03 ng	346662	Chrysene-d12	14.00	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	90
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	49
3	1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	47
4	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	38
5	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	38



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WABUT-3(0-2)

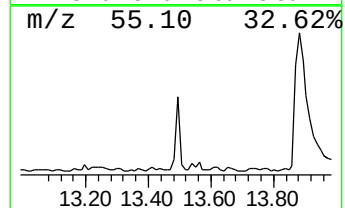
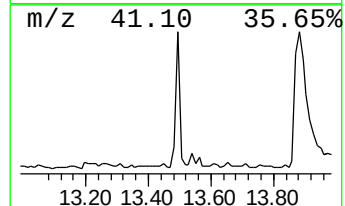
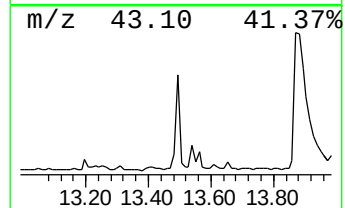
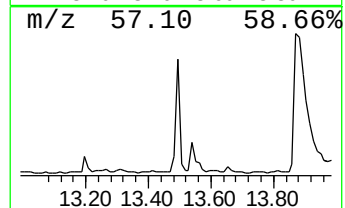
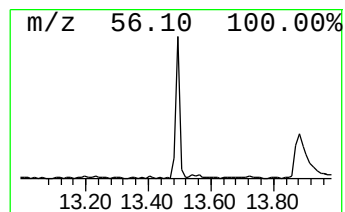
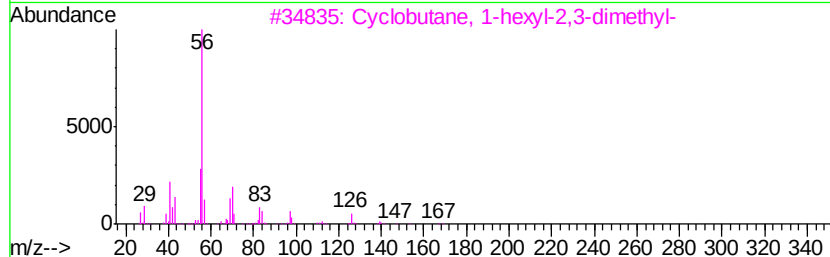
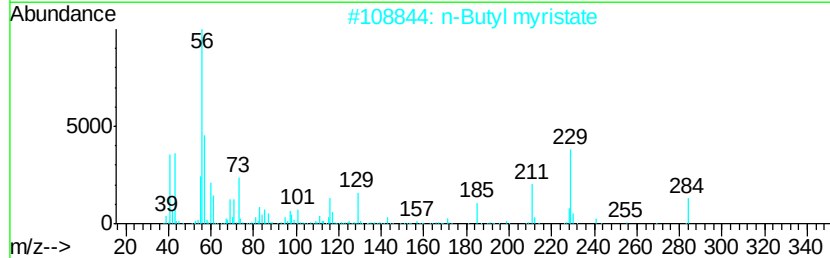
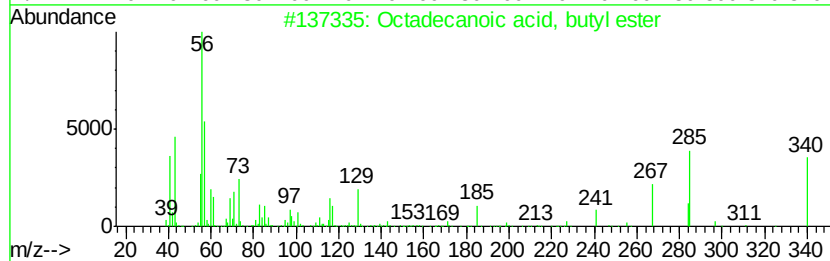
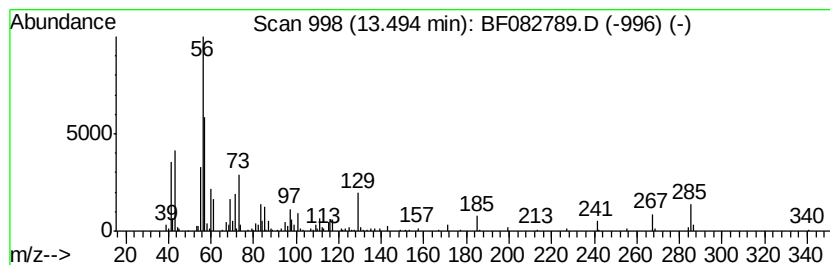
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.49	2.43 ng	277640	Chrysene-d12	14.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	94
2		n-Butyl myristate	284	C18H36O2	000110-36-1	64
3		Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	35
4		Pentadecane, 8-methylene-	224	C16H32	055668-09-2	32
5		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27



Data Path : Z:\HPCHEM1\BNA F\DATA\BF110815\
Data File : BF082789.D
Acq On : 7 Nov 2015 4:43
Operator : UM/IZ
Sample : G4257-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WABUT-3(0-2)

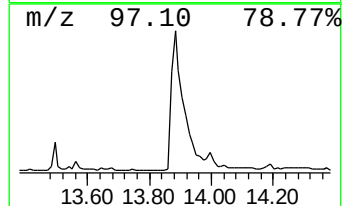
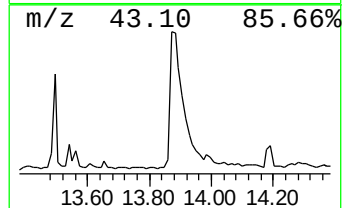
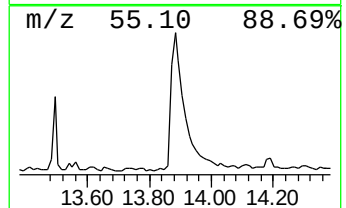
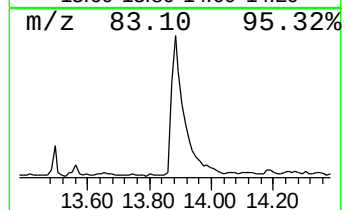
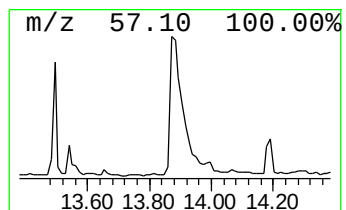
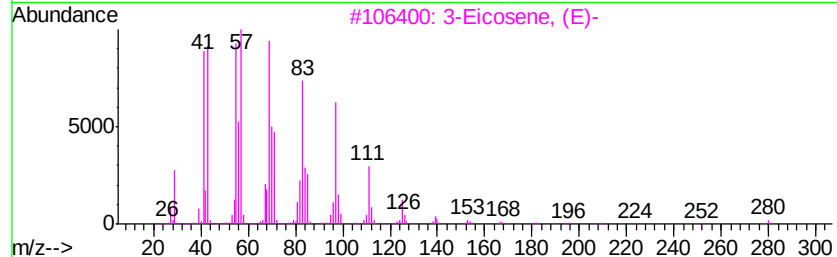
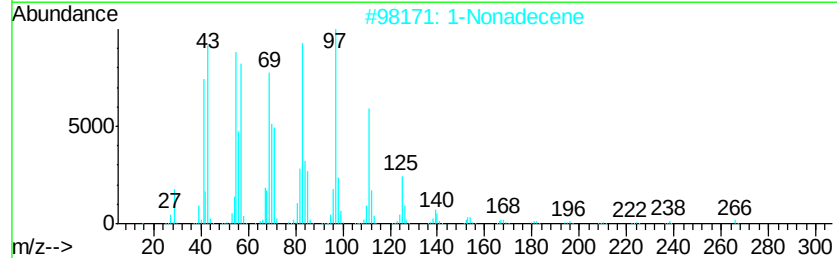
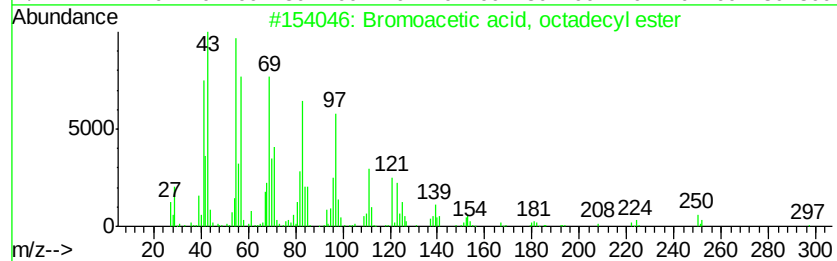
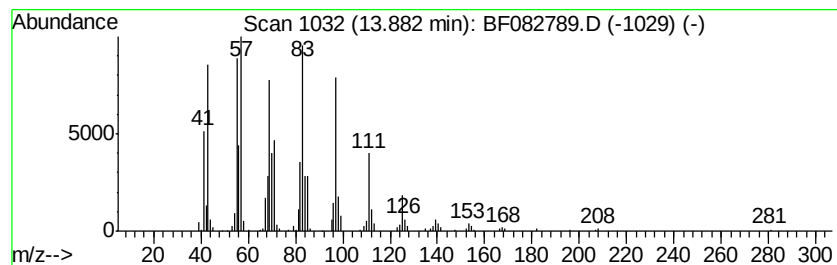
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Bromoacetic acid, octadecyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	10.05 ng	1148390	Chrysene-d12	14.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
2		1-Nonadecene	266	C19H38	018435-45-5	91
3		3-Eicosene, (E)-	280	C20H40	074685-33-9	91
4		Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	91
5		2- Chloropropionic acid, pentade...	318	C18H35ClO2	1000292-44-1	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF110815\
Data File : BF082789.D
Acq On : 7 Nov 2015 4:43
Operator : UM/IZ
Sample : G4257-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WABUT-3(0-2)

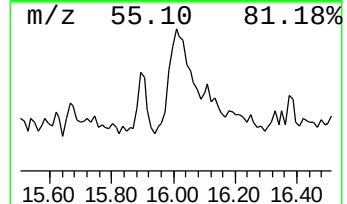
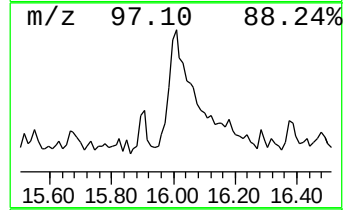
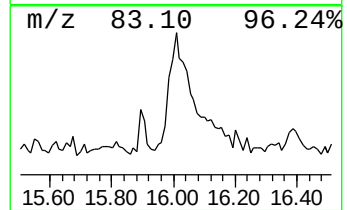
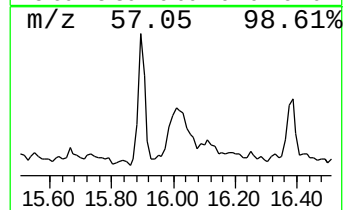
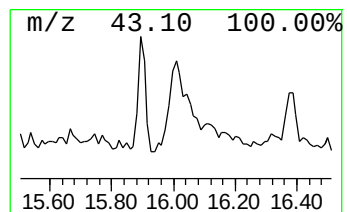
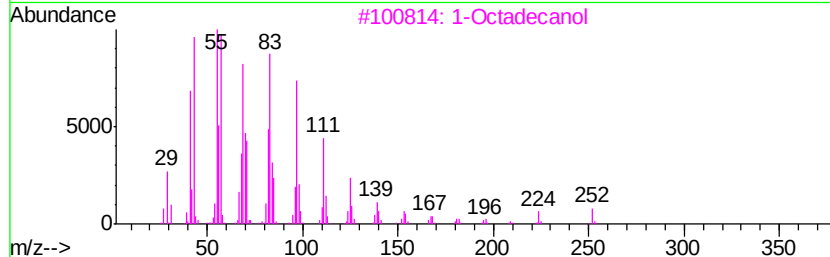
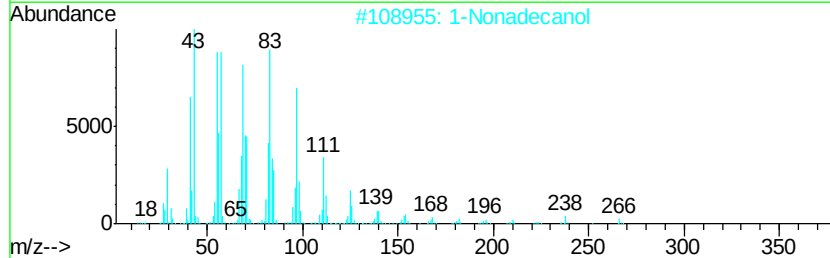
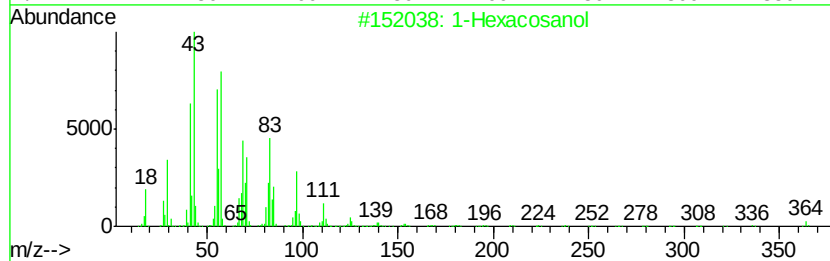
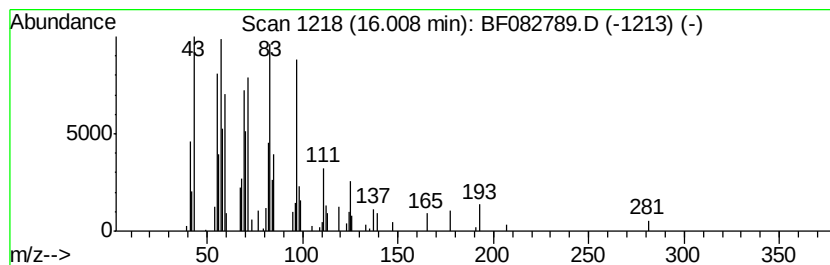
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Hexacosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.01	2.49 ng	228366	Perylene-d12	15.43

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexacosanol	382	C26H54O	000506-52-5	83
2		1-Nonadecanol	284	C19H40O	001454-84-8	60
3		1-Octadecanol	270	C18H38O	000112-92-5	60
4		3-Eicosene, (E)-	280	C20H40	074685-33-9	58
5		1,2-Octadecanediol	286	C18H38O2	020294-76-2	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110815\
Data File : BF082789.D
Acq On : 7 Nov 2015 4:43
Operator : UM/IZ
Sample : G4257-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WABUT-3(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	45.6	ng	3478780	1	6.84	1526420	20.0
unknown6.61	6.61	78.6	ng	6001340	1	6.84	1526420	20.0
Octadecane	10.81	2.0	ng	253870	4	11.37	2530530	20.0
n-Hexadecanoic acid	11.91	2.7	ng	345648	4	11.37	2530530	20.0
Hexadecanoic acid...	12.79	3.0	ng	346662	5	14.00	2285560	20.0
Octadecanoic acid...	13.49	2.4	ng	277640	5	14.00	2285560	20.0
Bromoacetic acid,...	13.88	10.1	ng	1148390	5	14.00	2285560	20.0
1-Hexacosanol	16.01	2.5	ng	228366	6	15.43	1836030	20.0