

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102115\
 Data File : BF082426.D
 Acq On : 22 Oct 2015 2:41
 Operator : UM/IZ
 Sample : G4116-03
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 NB3-02(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	255	rBV	842926	1406315	53.22%	6.039%
2	5.371	280	283	285	rBV	1917590	2316831	87.68%	9.948%
3	5.771	316	318	320	rBV	20100	27869	1.05%	0.120%
4	6.412	371	374	377	rBV	1692766	2121281	80.27%	9.109%
5	6.537	383	385	388	rBV	2499885	2334410	88.34%	10.024%
6	6.766	403	405	408	rBV	585830	527159	19.95%	2.264%
7	6.926	416	419	421	rBV	2104563	1982715	75.03%	8.514%
8	7.337	452	455	458	rBV	1136749	1344119	50.87%	5.772%
9	8.057	515	518	520	rBV	806779	687589	26.02%	2.952%
10	9.143	610	613	615	rBV	2216545	2642518	100.00%	11.347%
11	9.532	645	647	650	rBV	439304	423796	16.04%	1.820%
12	9.818	669	672	674	rBV	614842	747225	28.28%	3.209%
13	10.240	708	709	711	rVB	35504	29970	1.13%	0.129%
14	10.606	738	741	743	rBV	1471078	1514349	57.31%	6.502%
15	10.721	749	751	755	rVB	41816	61340	2.32%	0.263%
16	11.166	788	790	791	rBV	41411	37370	1.41%	0.160%
17	11.303	799	802	804	rBV	505269	693375	26.24%	2.977%
18	11.829	846	848	854	rVB	96956	108080	4.09%	0.464%
19	12.515	905	908	910	rBV	32437	36414	1.38%	0.156%
20	12.744	926	928	930	rBV	25843	27705	1.05%	0.119%
21	12.892	938	941	943	rBV	2270720	2175522	82.33%	9.341%
22	13.795	1017	1020	1027	rBV	84239	151180	5.72%	0.649%
23	13.955	1031	1034	1036	rBV	402329	533810	20.20%	2.292%
24	14.127	1046	1049	1055	rBV6	9870	28873	1.09%	0.124%
25	14.447	1074	1077	1084	rBV3	40105	112331	4.25%	0.482%
26	14.835	1109	1111	1113	rVB	30604	34599	1.31%	0.149%
27	14.904	1115	1117	1120	rBV	26958	26611	1.01%	0.114%
28	15.007	1124	1126	1131	rBV	17887	31151	1.18%	0.134%
29	15.087	1131	1133	1134	rBV	36061	43595	1.65%	0.187%
30	15.121	1134	1136	1138	rBV3	18492	34846	1.32%	0.150%
31	15.418	1159	1162	1170	rVB	367109	529049	20.02%	2.272%
32	15.635	1178	1181	1183	rBV	31760	43104	1.63%	0.185%
33	15.852	1197	1200	1203	rBV	42326	62493	2.36%	0.268%
34	16.595	1262	1265	1269	rVB	29133	48878	1.85%	0.210%

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

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

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35	16.870	1286	1289	1292	rVB2	17793	33173	1.26%	0.142%
36	17.327	1326	1329	1338	rVB6	13772	53153	2.01%	0.228%
37	17.510	1342	1345	1349	rVB2	29546	62061	2.35%	0.266%
38	17.921	1377	1381	1385	rBV4	11143	27896	1.06%	0.120%
39	18.024	1387	1390	1398	rVB7	9226	27829	1.05%	0.119%
40	18.276	1408	1412	1417	rVB3	20568	63170	2.39%	0.271%
41	18.698	1445	1449	1453	rBV3	16921	49022	1.86%	0.210%
42	19.236	1492	1496	1502	rVB10	13226	46107	1.74%	0.198%

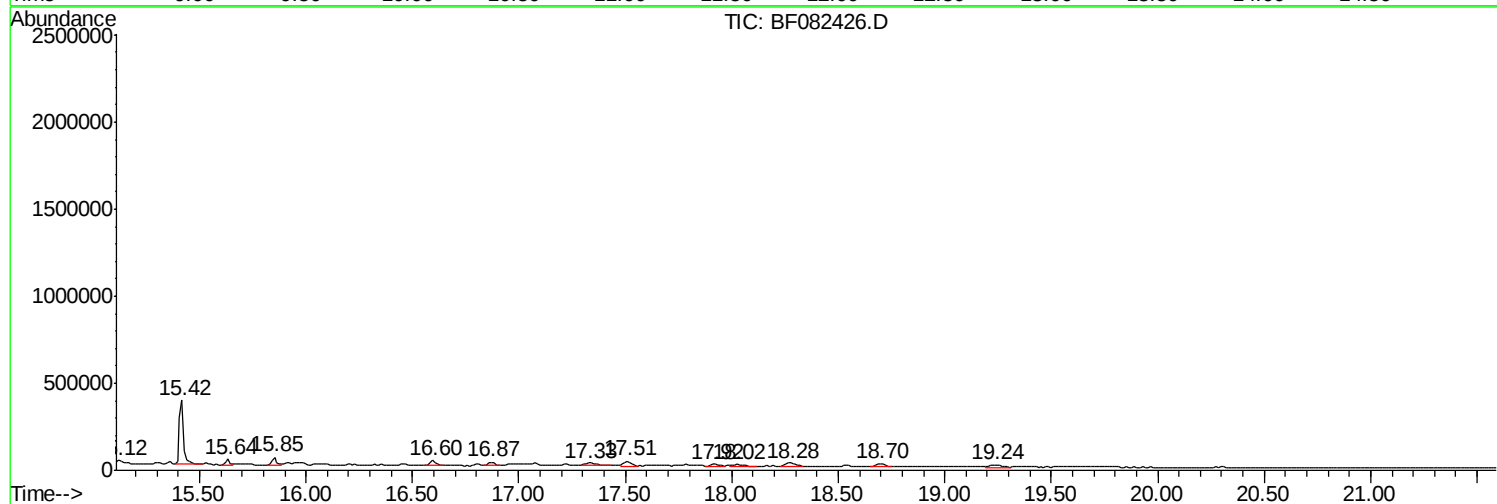
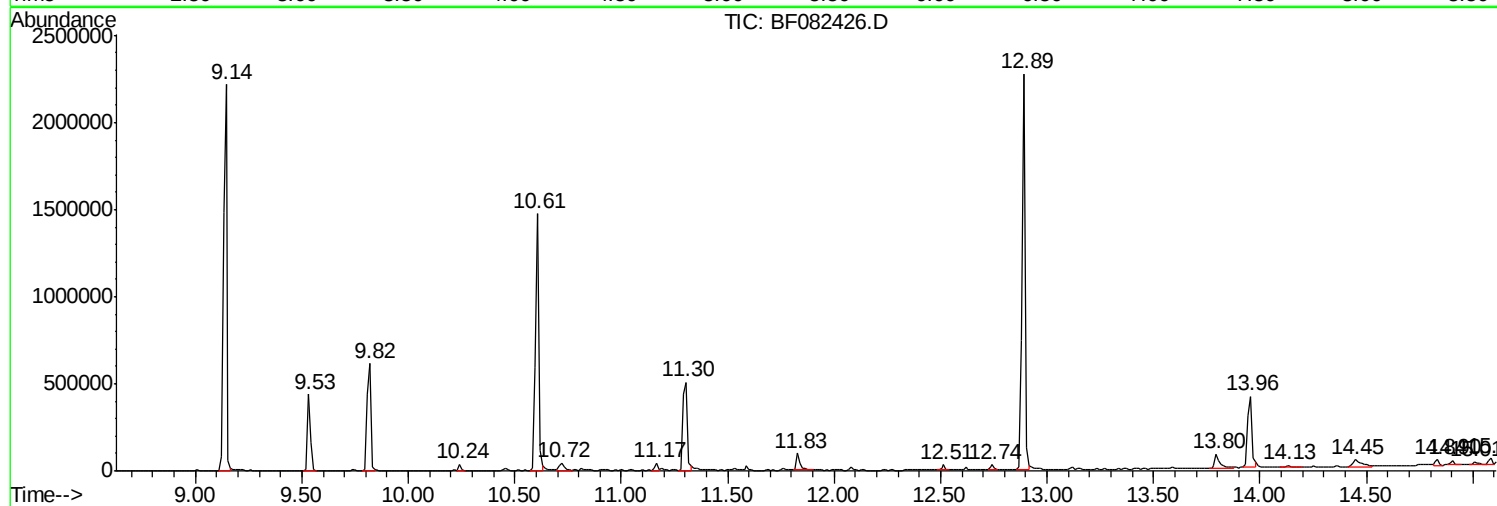
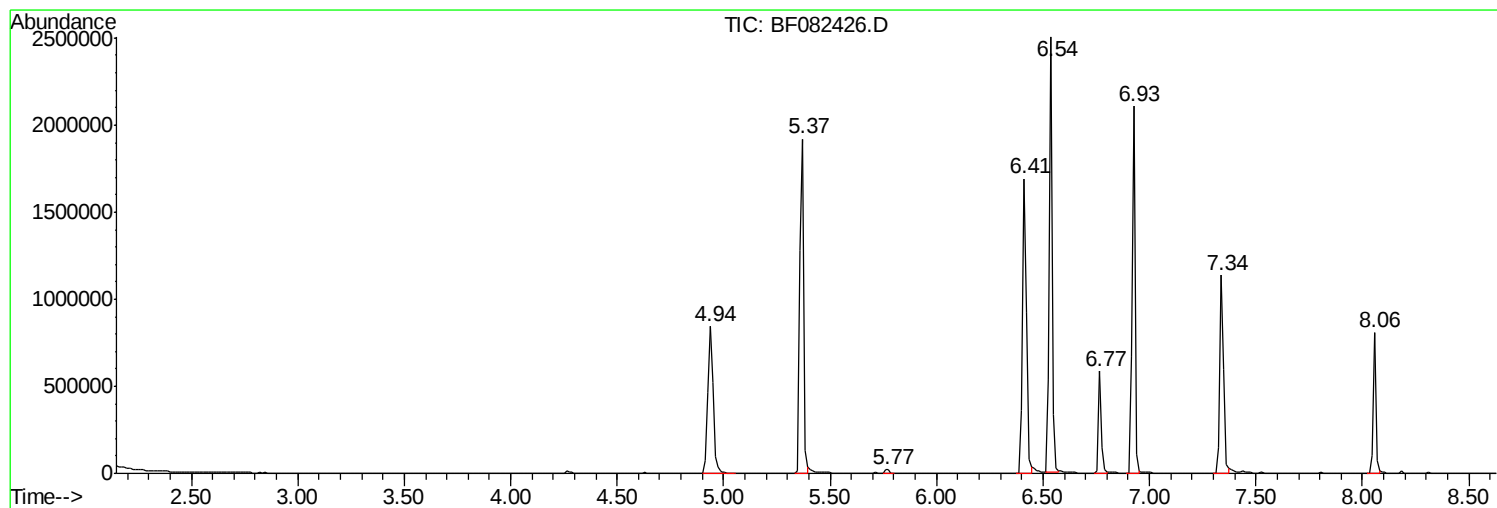
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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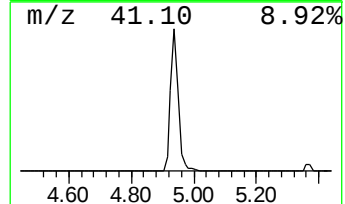
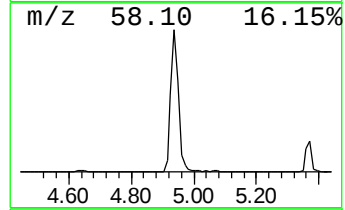
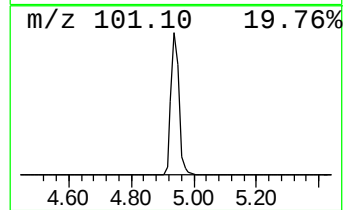
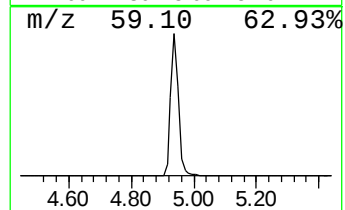
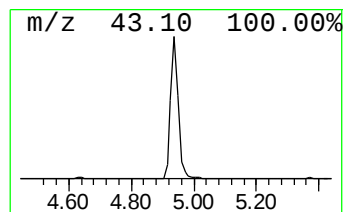
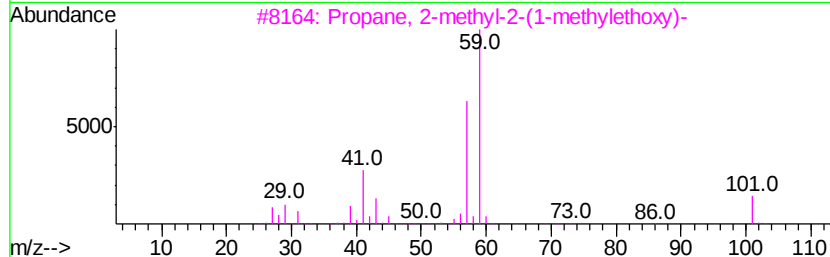
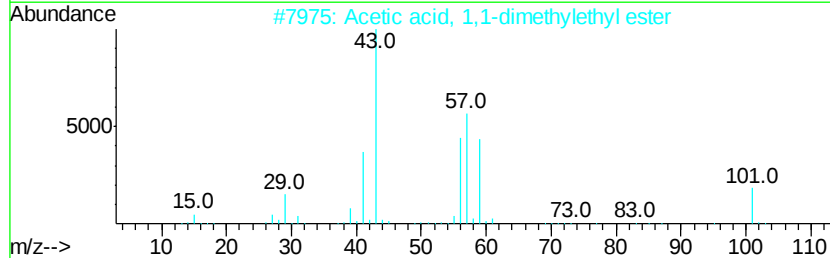
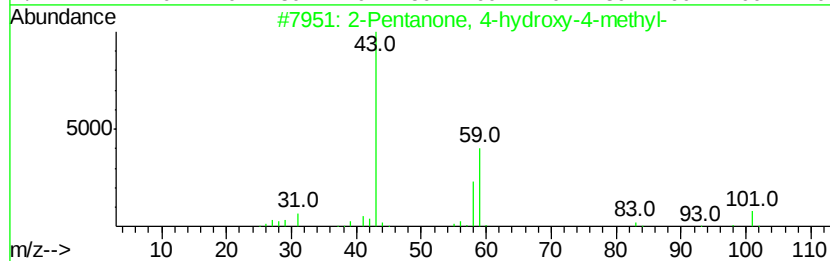
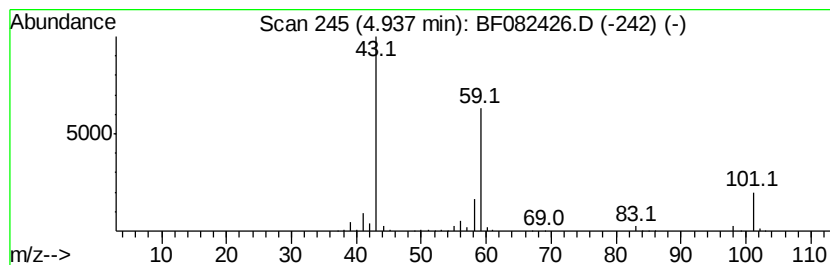
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.94	53.35 ng	1406320	1,4-Dichlorobenzene-d4	6.77

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23



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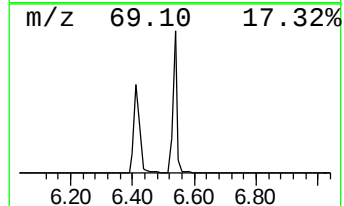
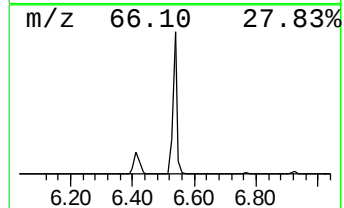
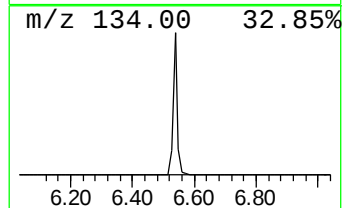
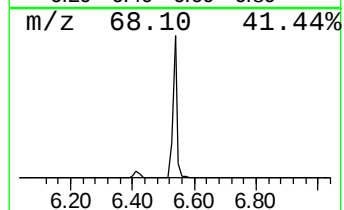
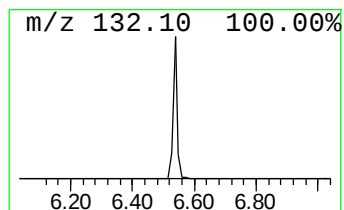
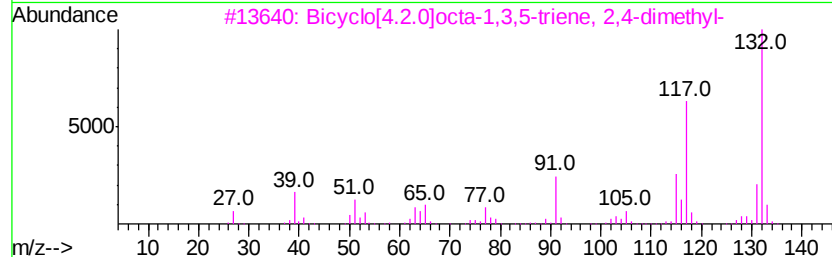
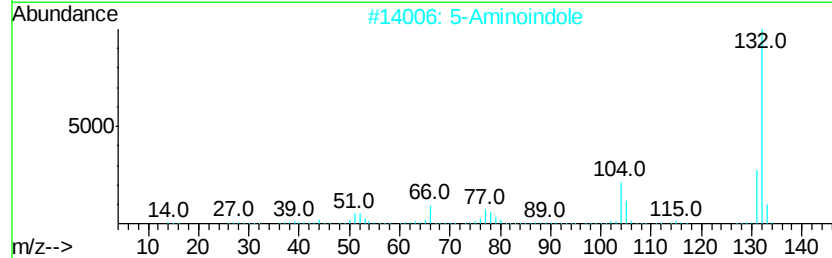
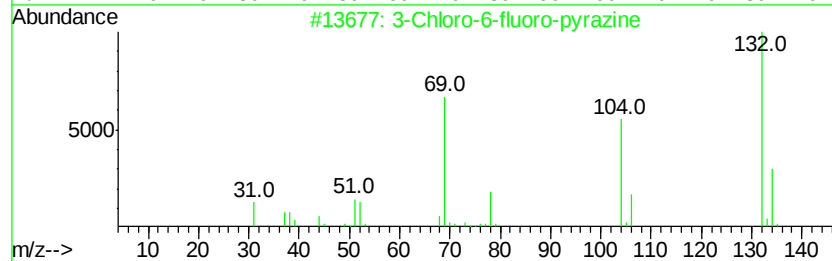
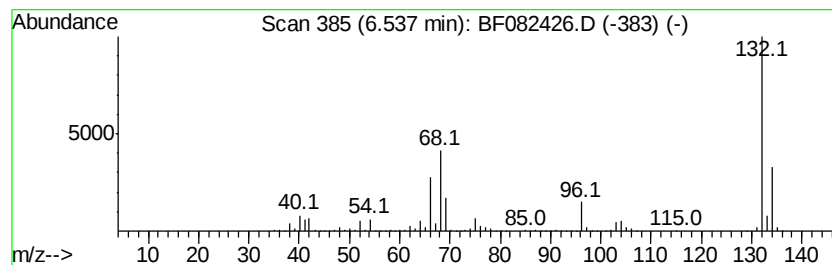
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.54 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.54	88.57 ng	2334410	1,4-Dichlorobenzene-d4	6.77

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4			Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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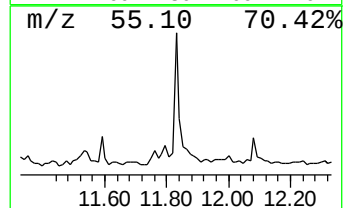
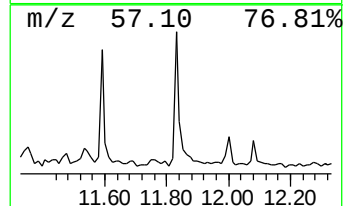
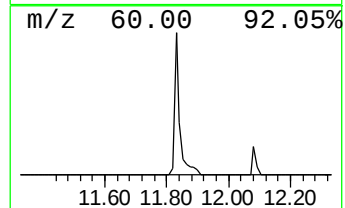
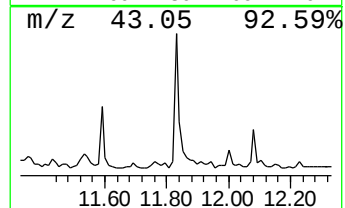
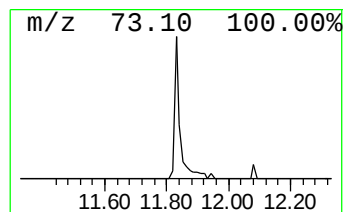
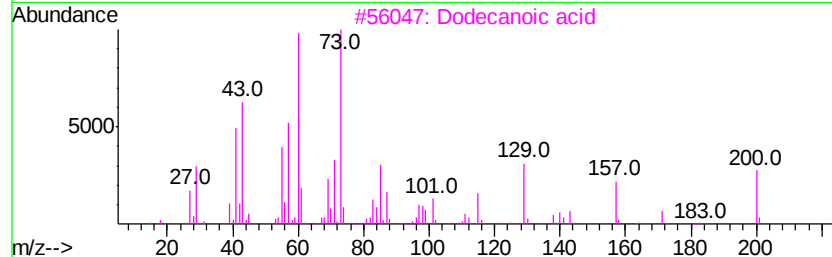
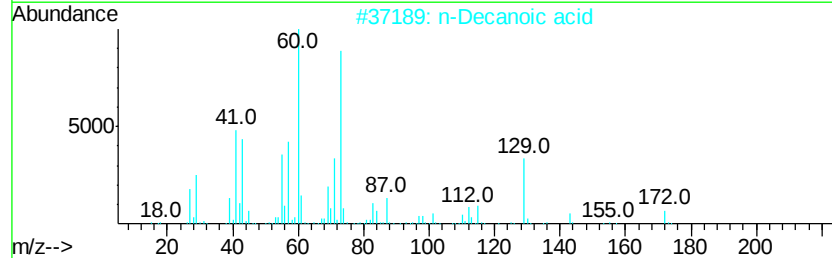
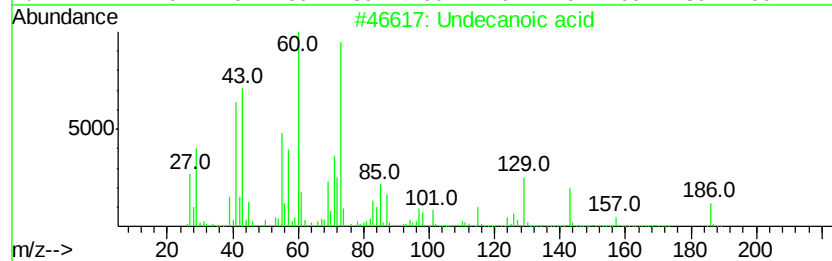
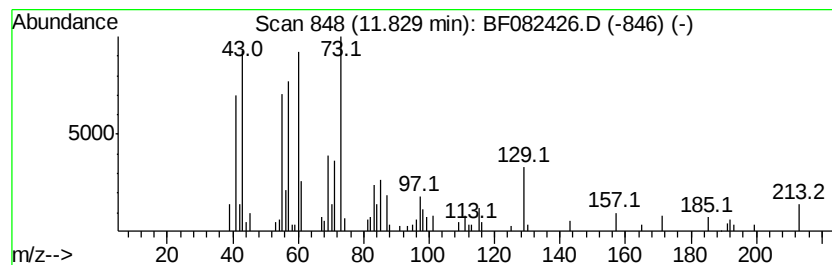
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Undecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.83	3.12 ng	108080	Phenanthrene-d10	11.30

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid		186	C11H22O2	000112-37-8	64
2	n-Decanoic acid		172	C10H20O2	000334-48-5	50
3	Dodecanoic acid		200	C12H24O2	000143-07-7	50
4	Octanoic Acid		144	C8H16O2	000124-07-2	47
5	.alpha.-D-Glucopyranose, 4-O-.be...		342	C12H22O11	014641-93-1	45



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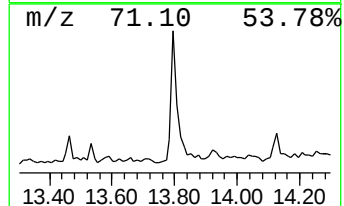
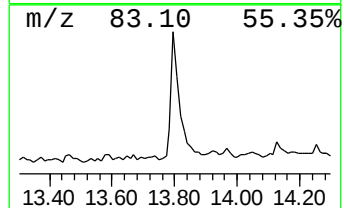
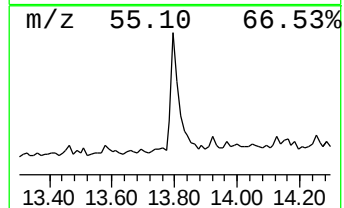
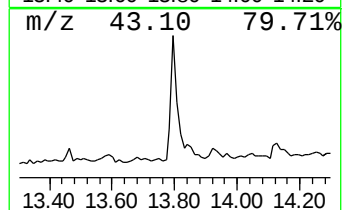
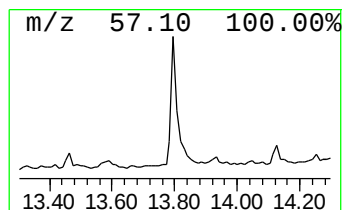
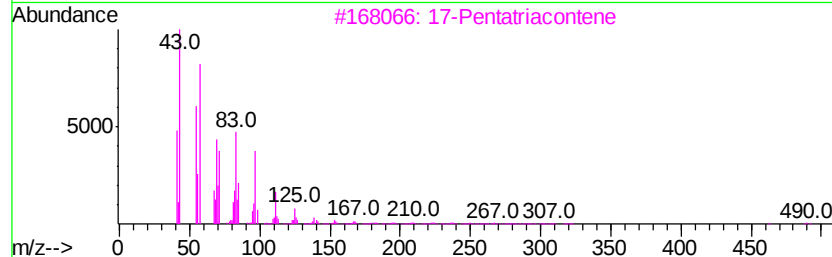
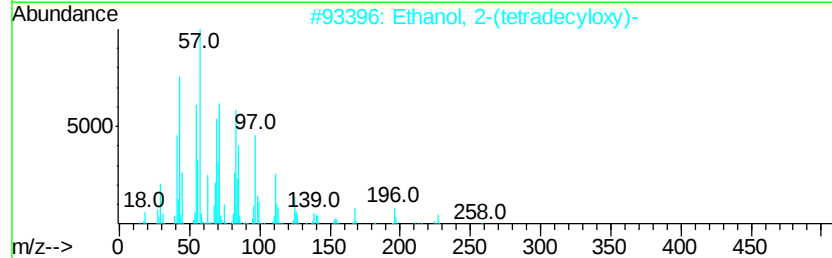
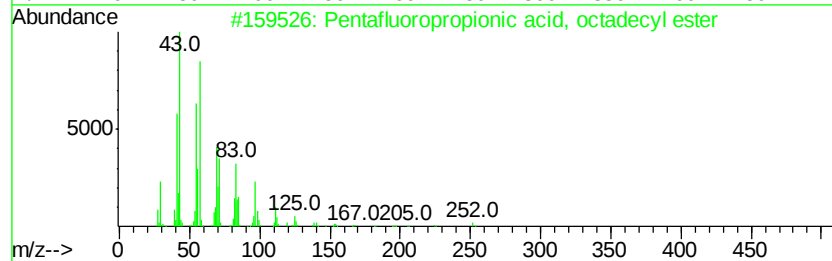
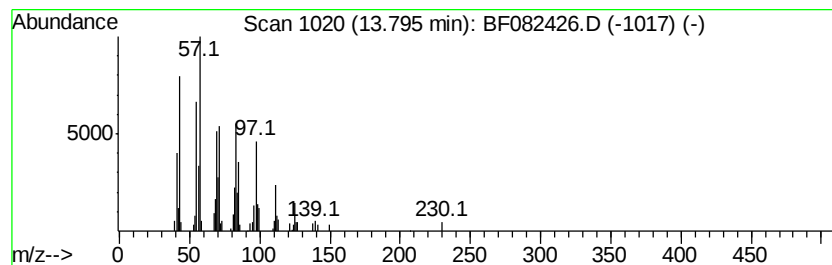
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Pentafluoropropionic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	5.66 ng	151180	Chrysene-d12	13.96

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	91
2		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
3		17-Pentatriacontene	491	C35H70	006971-40-0	90
4		Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	81
5		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	81



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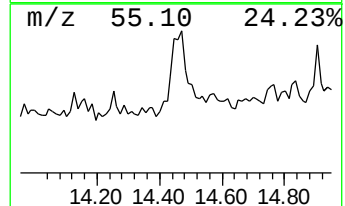
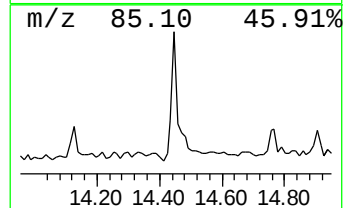
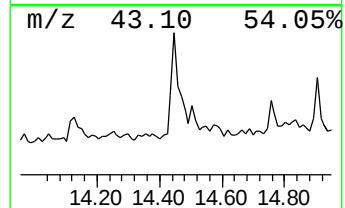
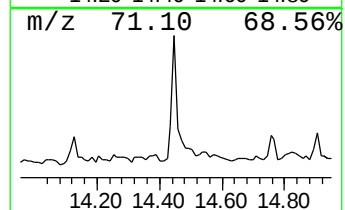
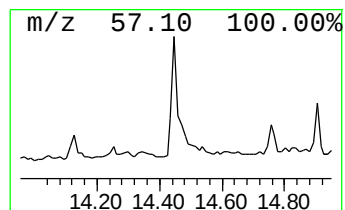
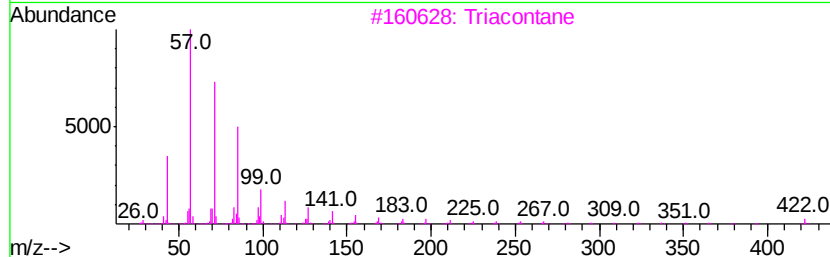
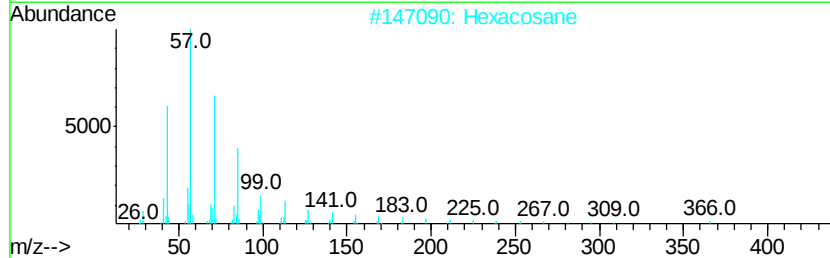
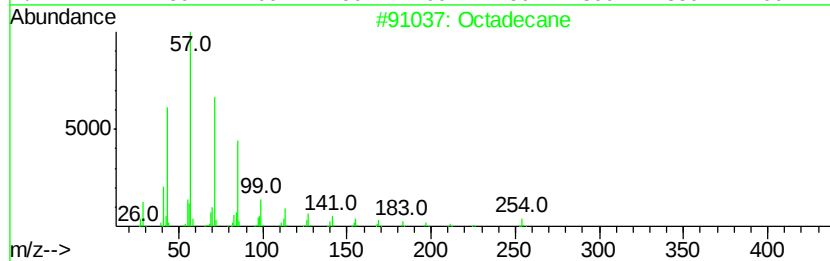
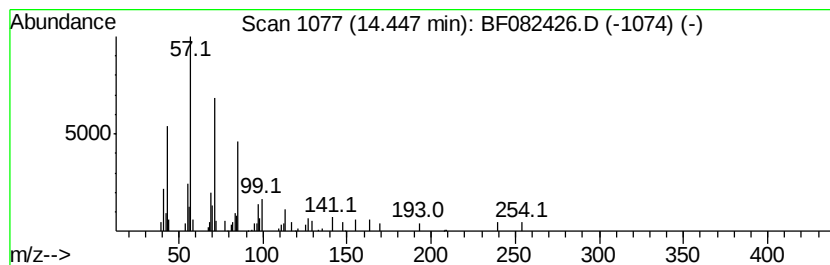
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.45	4.21 ng	112331	Chrysene-d12	13.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane	254	C18H38	000593-45-3	96
2		Hexacosane	366	C26H54	000630-01-3	90
3		triacontane	422	C30H62	000638-68-6	87
4		Heneicosane	296	C21H44	000629-94-7	87
5		Tetratriacontane	479	C34H70	014167-59-0	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102115\
Data File : BF082426.D
Acq On : 22 Oct 2015 2:41
Operator : UM/IZ
Sample : G4116-03
Misc :
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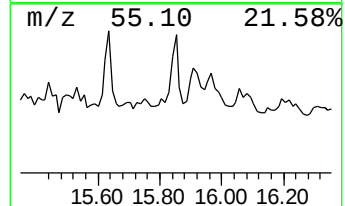
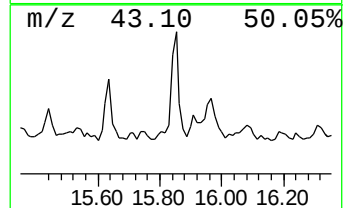
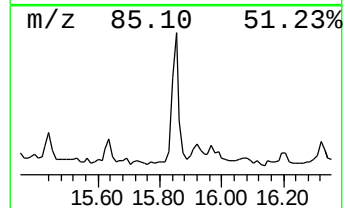
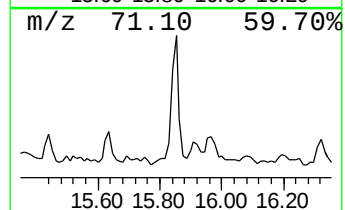
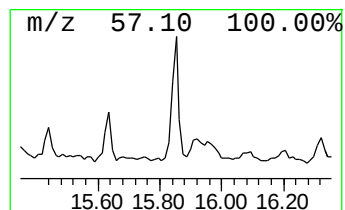
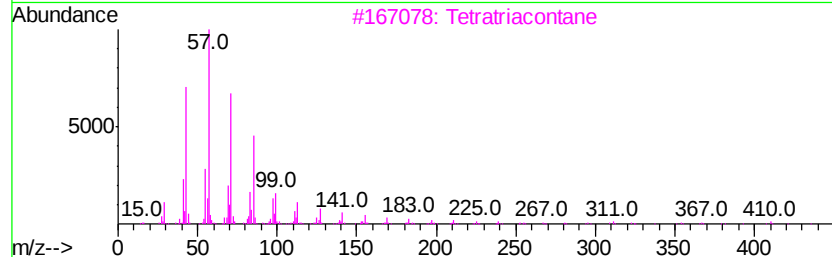
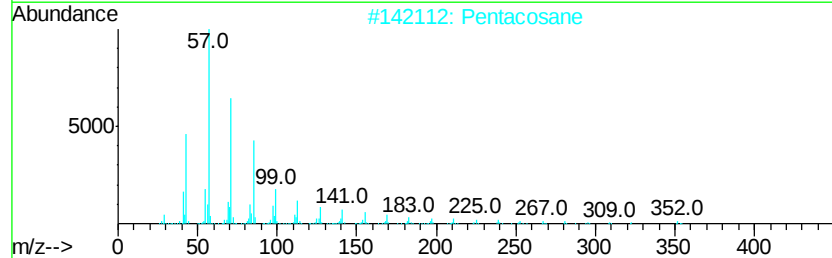
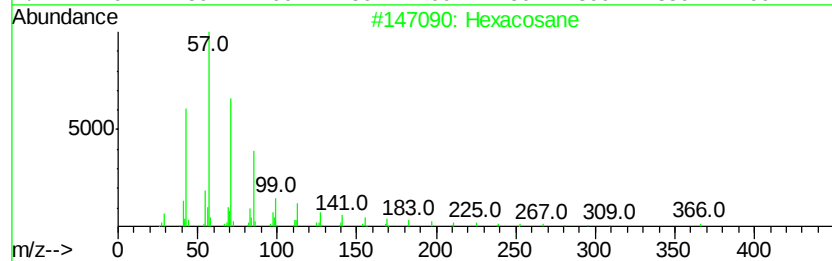
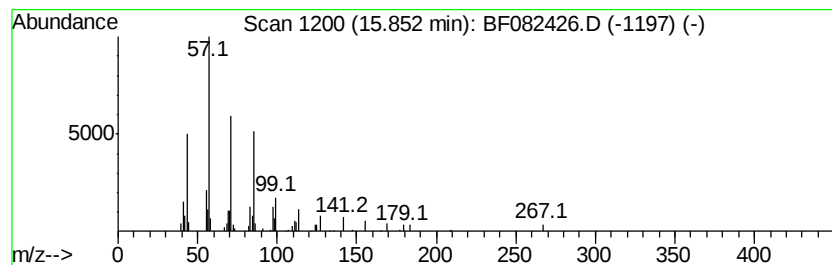
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ClientSampleId :
NB3-02(0-2)

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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 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.85	2.36 ng	62493	Perylene-d12	15.42	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	90
2	Pentacosane	352	C25H52	000629-99-2	90
3	Tetratriacontane	479	C34H70	014167-59-0	90
4	Octacosane	394	C28H58	000630-02-4	90
5	Octadecane	254	C18H38	000593-45-3	87



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102115\
Data File : BF082426.D
Acq On : 22 Oct 2015 2:41
Operator : UM/IZ
Sample : G4116-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB3-02(0-2)

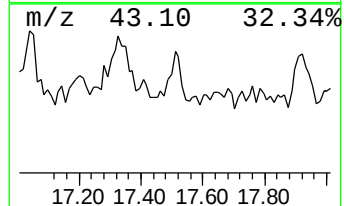
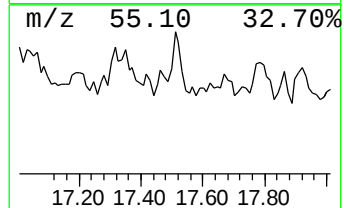
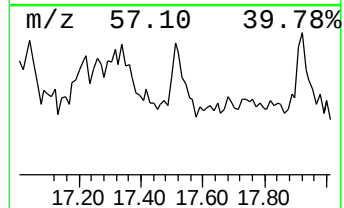
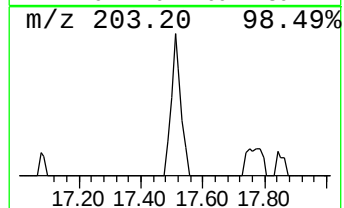
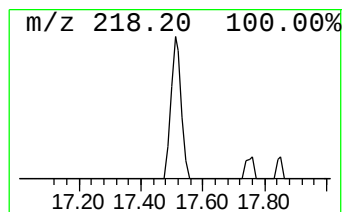
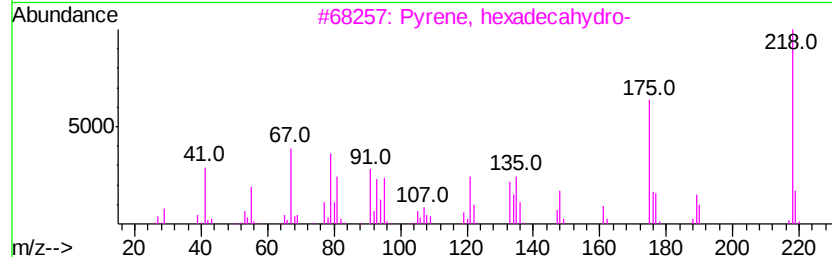
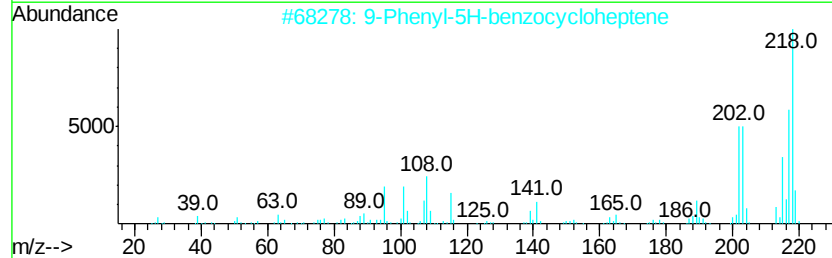
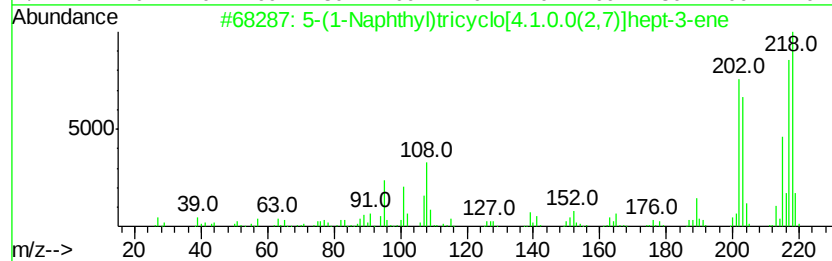
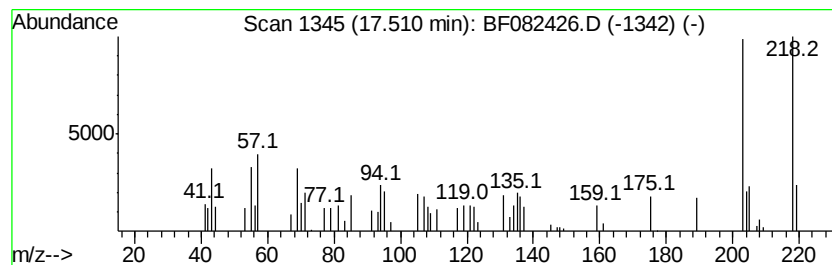
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown17.51 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.51	2.35 ng	62061	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-(1-Naphthyl)tricyclo[4.1.0.0(2...	218	C17H14	107729-05-5	43
2		9-Phenyl-5H-benzocycloheptene	218	C17H14	138089-71-1	38
3		Pvrene, hexadecahydro-	218	C16H26	002435-85-0	32
4		9,11-Dimethyltetracyclo[7.3.1.0(...	218	C16H26	053263-99-3	32
5		7b-Phenyl-2a,7b-dihydro-3H-cyclo...	218	C17H14	138089-70-0	28



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102115\
Data File : BF082426.D
Acq On : 22 Oct 2015 2:41
Operator : UM/IZ
Sample : G4116-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB3-02(0-2)

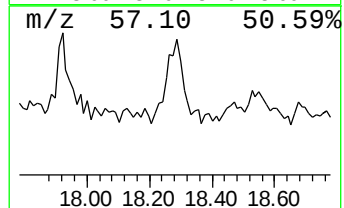
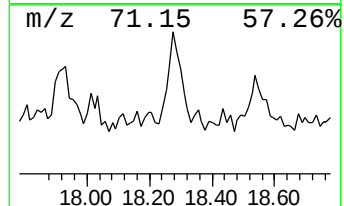
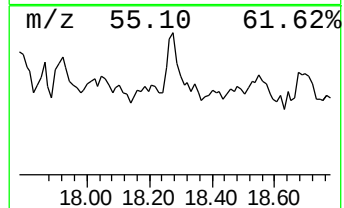
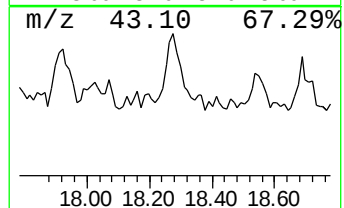
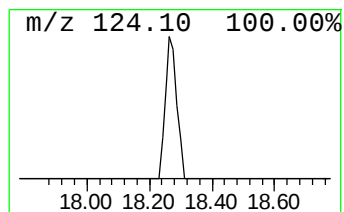
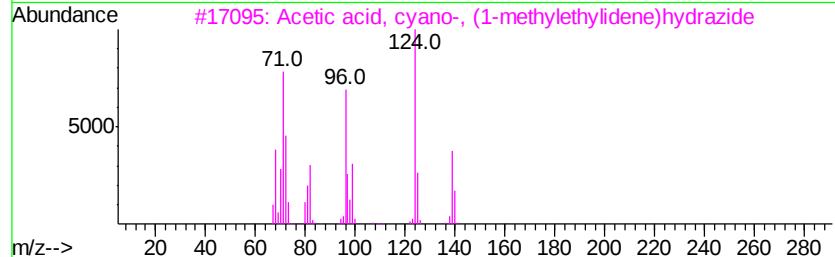
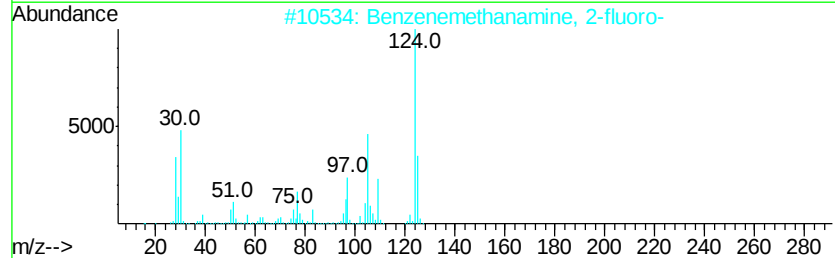
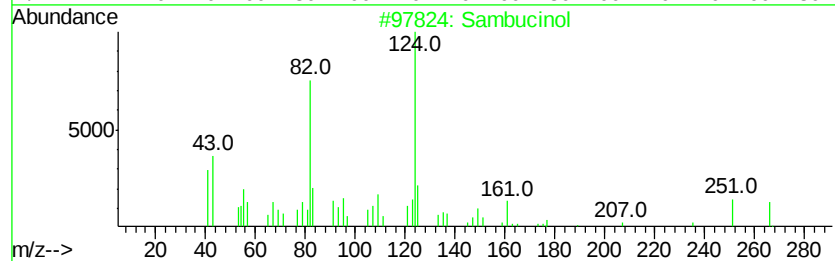
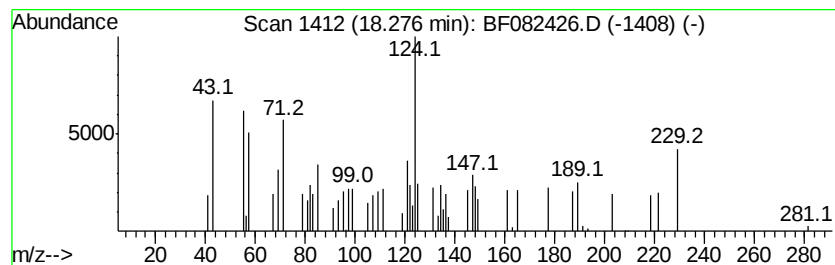
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown18.28 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.28	2.39 ng	63170	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sambucinol	266	C15H22O4	090044-33-0	22
2		Benzenemethanamine, 2-fluoro-	125	C7H8FN	000089-99-6	10
3		Acetic acid, cyano-, (1-methylethylidene)hydrazide	139	C6H9N3O	004974-42-9	10
4		2,4-Diaminophenol	124	C6H8N2O	000095-86-3	9
5		Phenol, 2,6-diamino-	124	C6H8N2O	022440-82-0	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102115\
Data File : BF082426.D
Acq On : 22 Oct 2015 2:41
Operator : UM/IZ
Sample : G4116-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB3-02(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
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unknown6.54	6.54	88.6	ng	2334410	1	6.77	527159	20.0
Undecanoic acid	11.83	3.1	ng	108080	4	11.30	693375	20.0
Pentafluoropropio...	13.80	5.7	ng	151180	5	13.96	533810	20.0
Octadecane	14.45	4.2	ng	112331	5	13.96	533810	20.0
Hexacosane	15.85	2.4	ng	62493	6	15.42	529049	20.0
unknown17.51	17.51	2.4	ng	62061	6	15.42	529049	20.0
unknown18.28	18.28	2.4	ng	63170	6	15.42	529049	20.0