

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011915\
 Data File : BF076938.D
 Acq On : 19 Jan 2015 19:59
 Operator : IZ / TP
 Sample : G1110-02
 Misc : W
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BEM-8

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-BF011415.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	1.384	23	26	31	rBV2	7001	14048	1.24%	0.181%
2	1.453	31	32	43	rVB2	15274	35806	3.17%	0.462%
3	4.104	261	264	275	rBV	74850	166738	14.75%	2.150%
4	5.042	342	346	359	rVB	146862	297385	26.31%	3.835%
5	7.373	547	550	555	rBV	83940	156397	13.84%	2.017%
6	7.465	555	558	567	rVB	439185	697209	61.69%	8.991%
7	7.968	599	602	607	rVB	108190	178895	15.83%	2.307%
8	8.288	627	630	634	rBV	413714	727495	64.37%	9.382%
9	9.271	712	716	719	rBV	384979	569451	50.39%	7.344%
10	10.882	853	857	860	rBV	160205	242320	21.44%	3.125%
11	13.534	1085	1089	1092	rBV	758118	1130109	100.00%	14.574%
12	15.008	1215	1218	1222	rBV	162507	259650	22.98%	3.349%
13	15.923	1295	1298	1302	rBV	21642	30762	2.72%	0.397%
14	16.620	1357	1359	1361	rBV	12554	17875	1.58%	0.231%
15	16.677	1361	1364	1367	rVV	509088	625032	55.31%	8.061%
16	17.774	1458	1460	1463	rBV	238496	262714	23.25%	3.388%
17	18.757	1544	1546	1548	rBV2	16253	17867	1.58%	0.230%
18	20.003	1653	1655	1658	rVB	1021501	1116650	98.81%	14.401%
19	21.272	1761	1766	1769	rBV	267880	409177	36.21%	5.277%
20	21.660	1797	1800	1802	rBV	14771	18378	1.63%	0.237%
21	22.038	1831	1833	1836	rVB	15961	19970	1.77%	0.258%
22	22.415	1863	1866	1869	rVB	13333	17431	1.54%	0.225%
23	22.472	1869	1871	1874	rBV	35532	43977	3.89%	0.567%
24	22.781	1895	1898	1900	rBV	10846	16865	1.49%	0.217%
25	22.838	1900	1903	1908	rVB3	7908	12706	1.12%	0.164%
26	22.918	1908	1910	1913	rBV	209049	255733	22.63%	3.298%
27	23.135	1927	1929	1931	rBV2	7934	11962	1.06%	0.154%
28	23.501	1958	1961	1962	rBV3	8278	12929	1.14%	0.167%
29	23.535	1962	1964	1966	rVB	11298	17061	1.51%	0.220%
30	23.798	1983	1987	1990	rBV3	20619	40656	3.60%	0.524%
31	23.855	1990	1992	1998	rVB5	7853	16559	1.47%	0.214%
32	24.106	2011	2014	2019	rVB3	9167	18312	1.62%	0.236%
33	24.392	2036	2039	2044	rVB6	5338	13129	1.16%	0.169%
34	24.484	2044	2047	2051	rVV4	34367	73753	6.53%	0.951%

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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	24.552	2051	2053	2058	rVB4	13812	29271	2.59%	0.377%
36	24.895	2078	2083	2088	rBV7	13254	32083	2.84%	0.414%
37	26.084	2183	2187	2191	rBV4	10399	30830	2.73%	0.398%
38	26.781	2241	2248	2253	rBV3	37311	116922	10.35%	1.508%

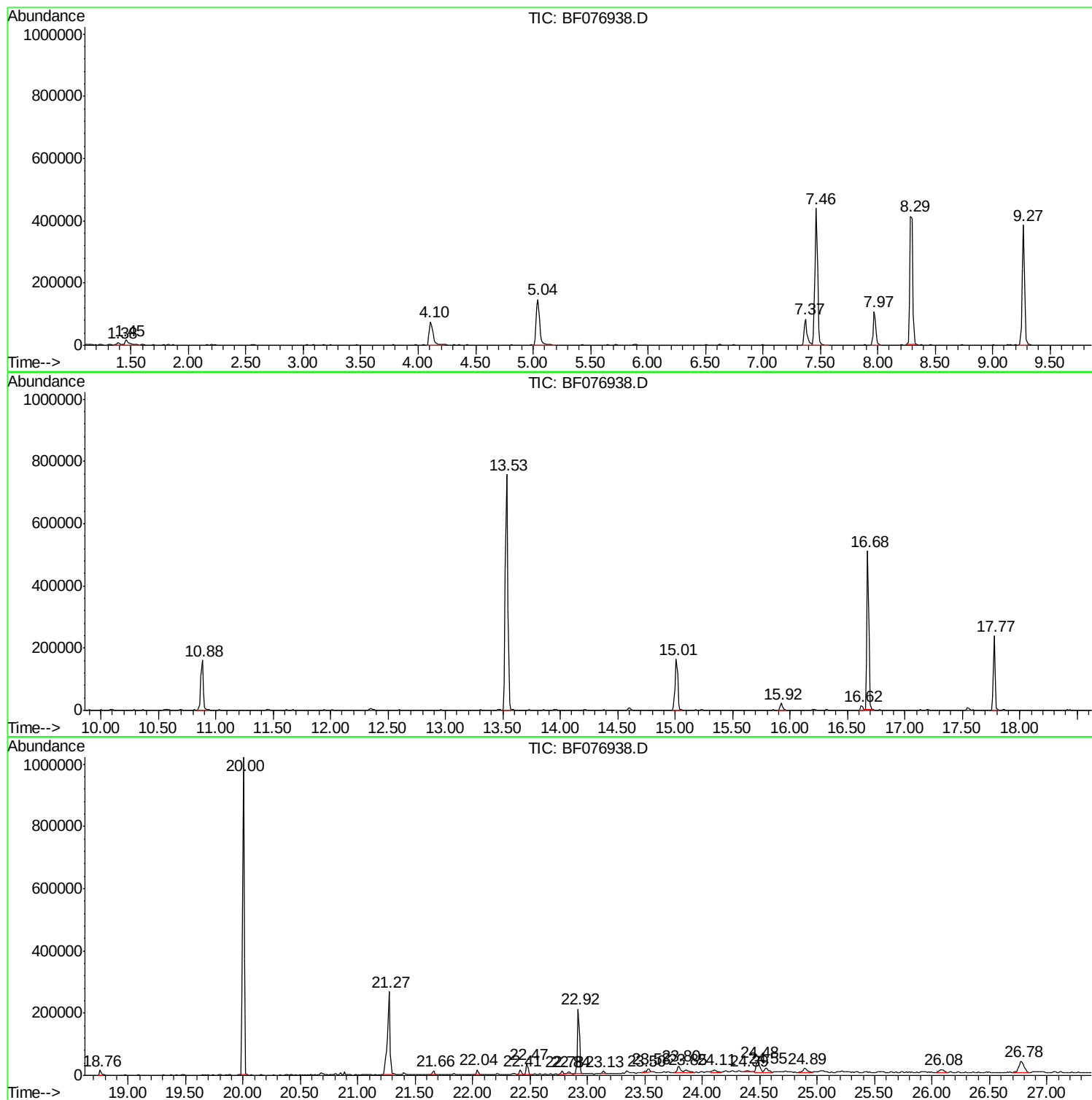
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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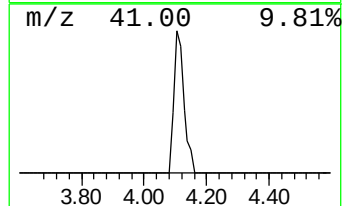
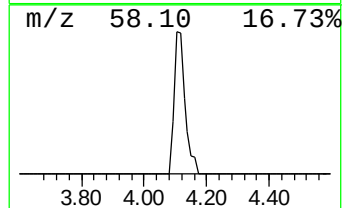
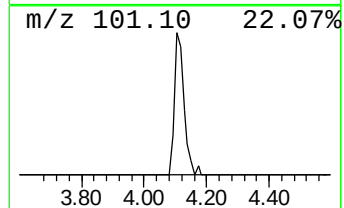
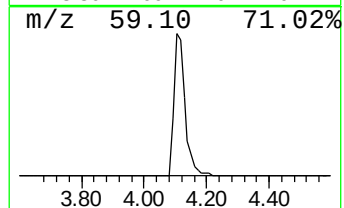
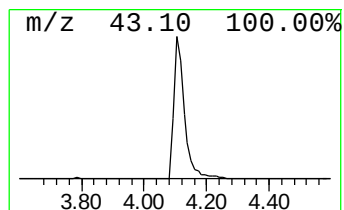
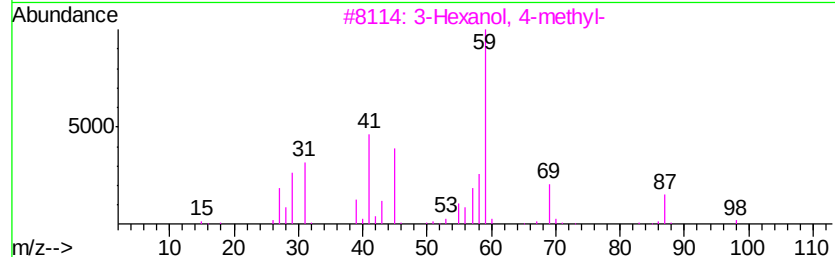
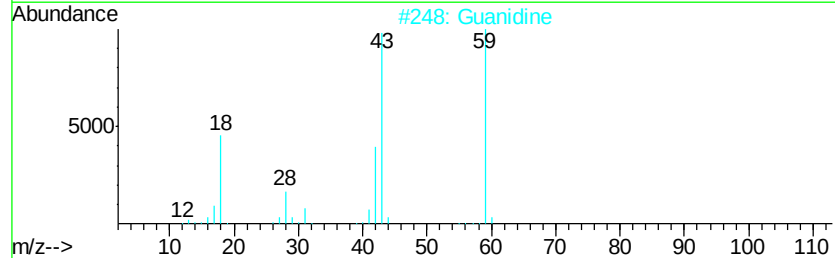
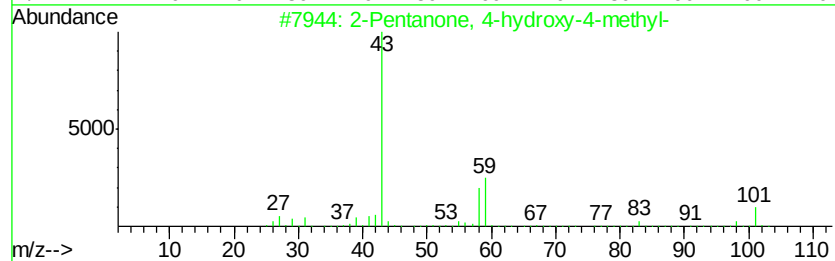
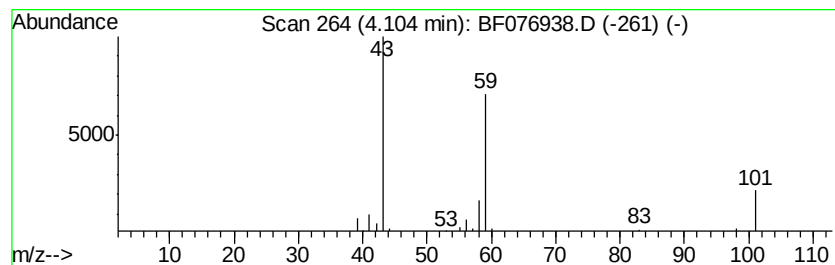
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.10	18.64 ng	166738	1,4-Dichlorobenzene-d4	7.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Guanidine	59	CH5N3	000113-00-8	43
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9



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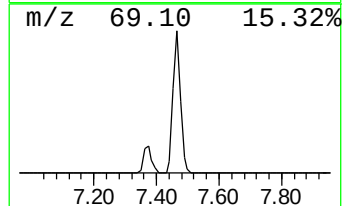
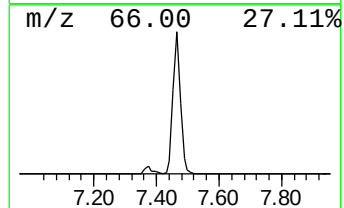
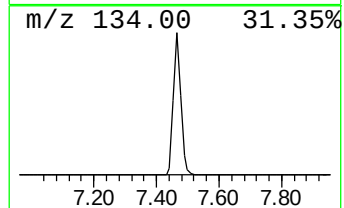
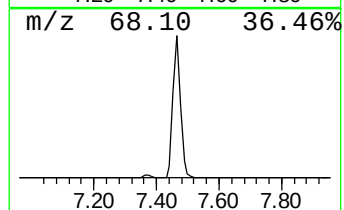
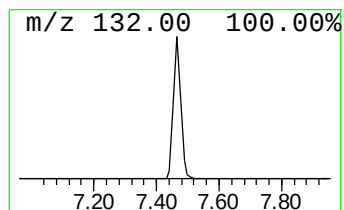
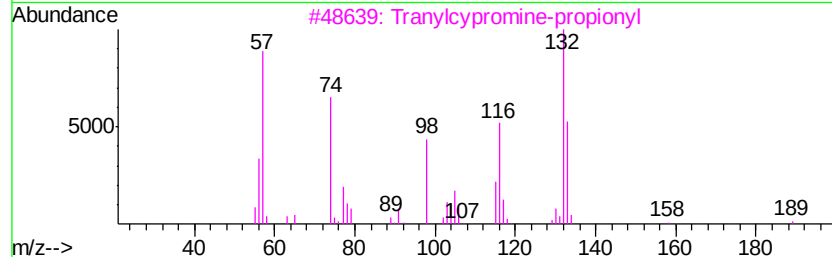
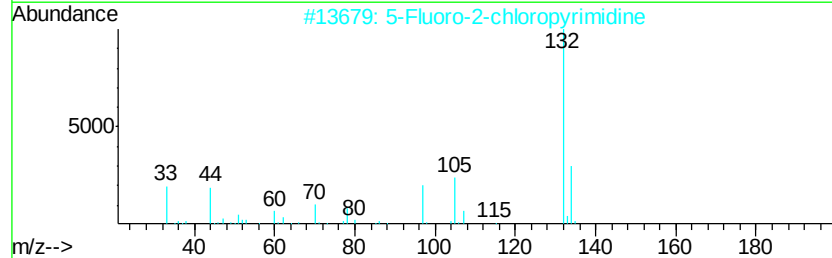
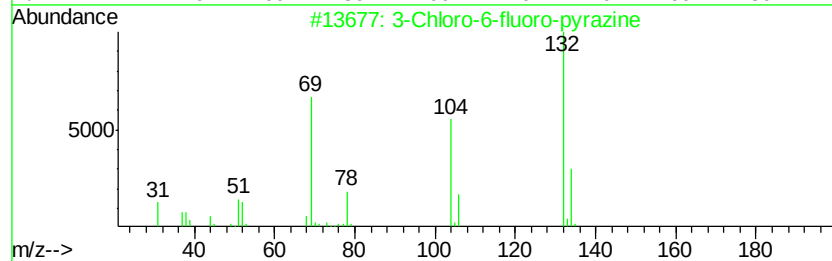
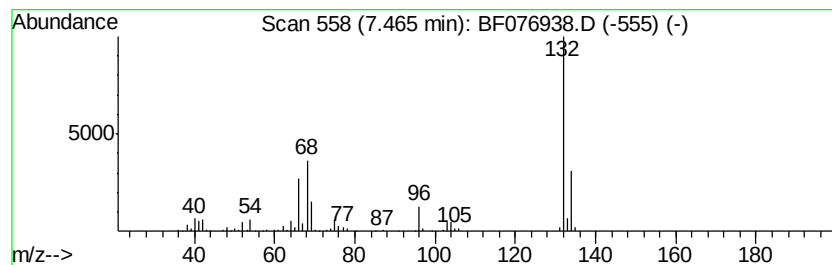
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown7.46 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.46	77.95 ng	697209	1,4-Dichlorobenzene-d4	7.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	25
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		2H-Cyclopentadlpyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9



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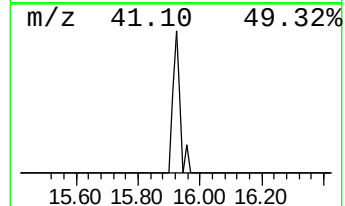
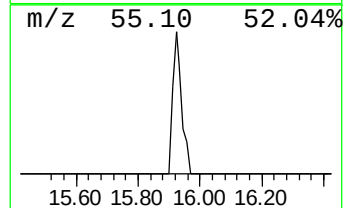
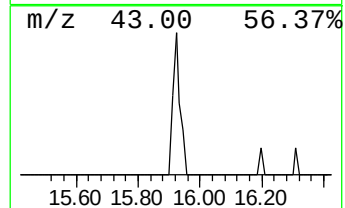
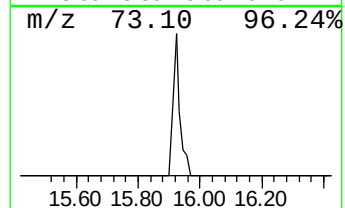
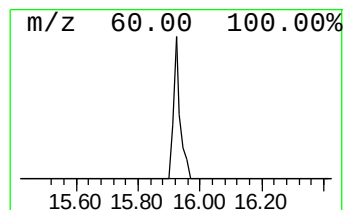
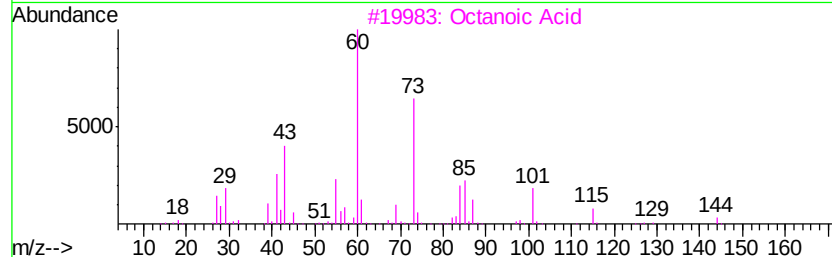
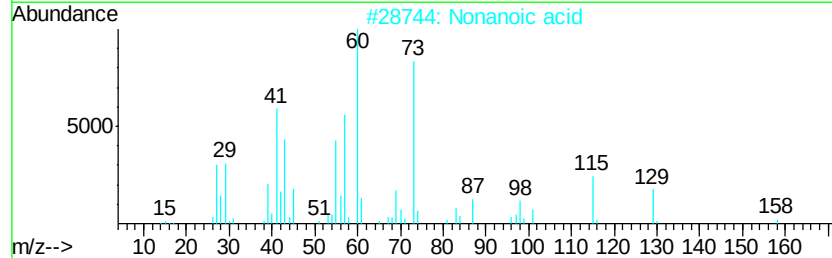
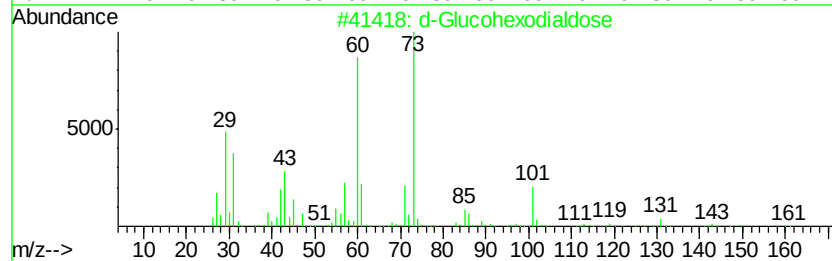
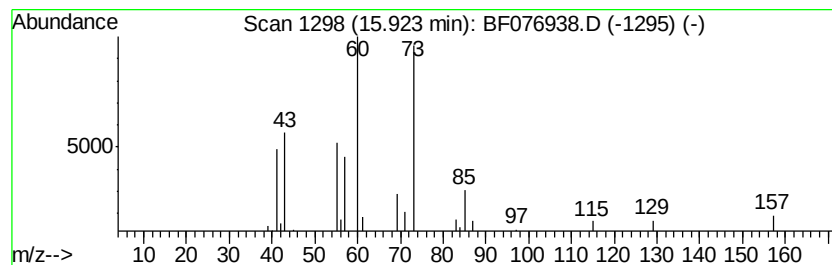
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 unknown15.92 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.
15.92	2.37 ng	30762	Acenaphthene-d10		15.01
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	d-Glucohexodialdose	178	C6H10O6	1000149-19-1	40
2	Nonanoic acid	158	C9H18O2	000112-05-0	40
3	Octanoic Acid	144	C8H16O2	000124-07-2	40
4	Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	32
5	Octane	114	C8H18	000111-65-9	10



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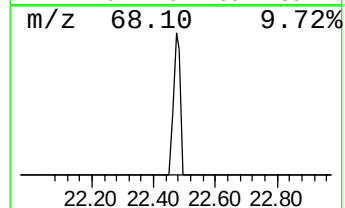
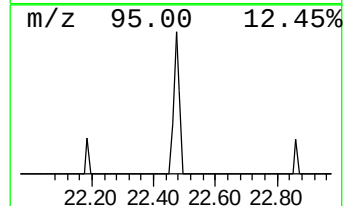
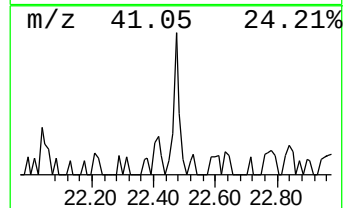
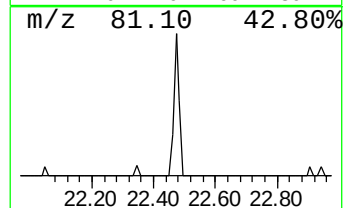
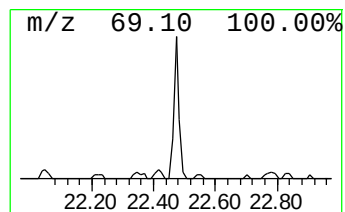
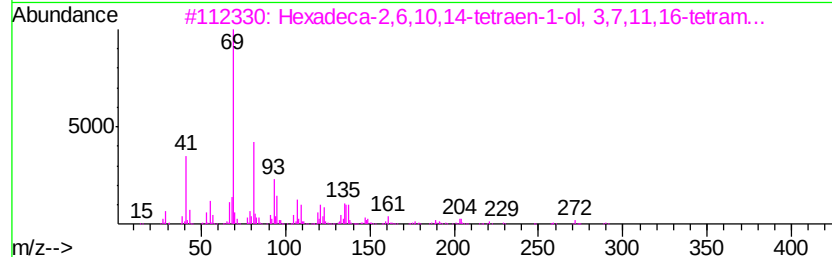
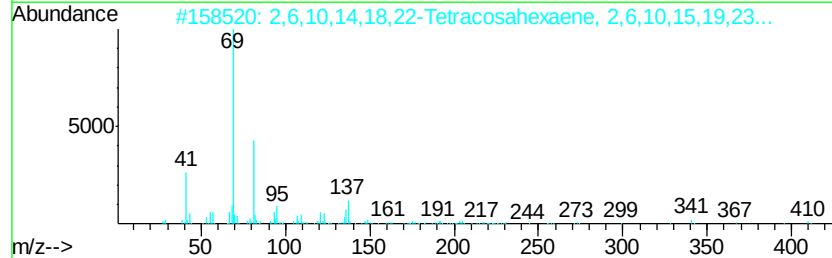
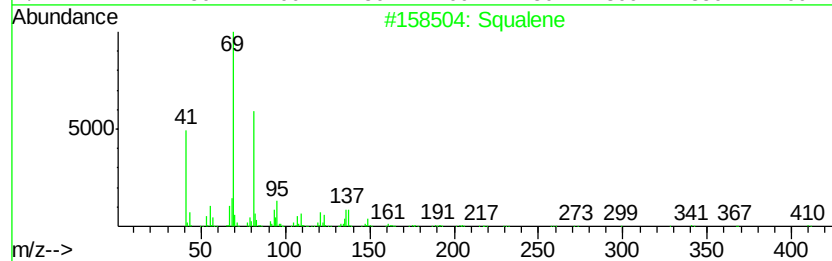
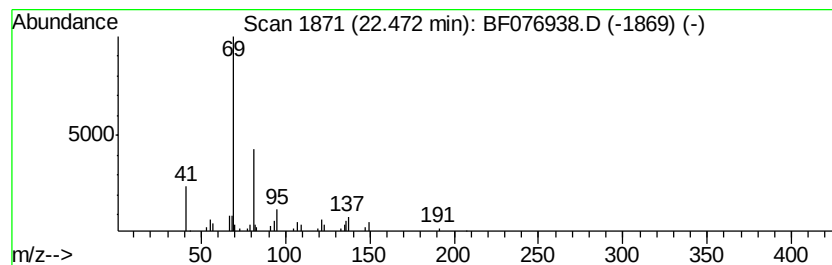
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.47	3.44 ng	43977	Perylene-d12	22.92
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Squalene	410 C30H50	007683-64-9	90
2	2,6,10,14,18,22-Tetracosahexaene...	410 C30H50	000111-02-4	83
3	Hexadeca-2,6,10,14-tetraen-1-ol,...	290 C20H34O	007614-21-3	78
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222 C15H26O	004602-84-0	72
5	7,11-Dimethyldodeca-2,6,10-trien...	208 C14H24O	125529-10-4	56



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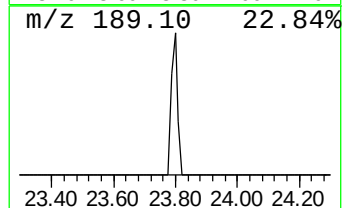
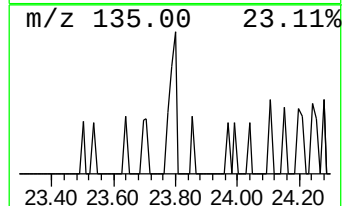
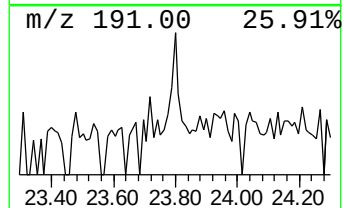
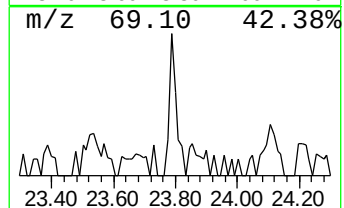
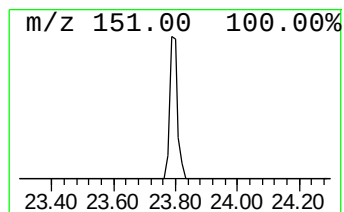
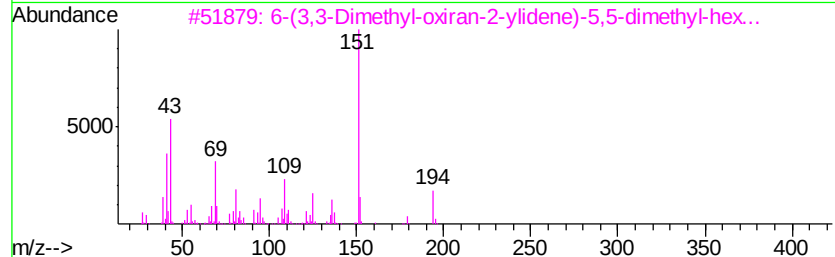
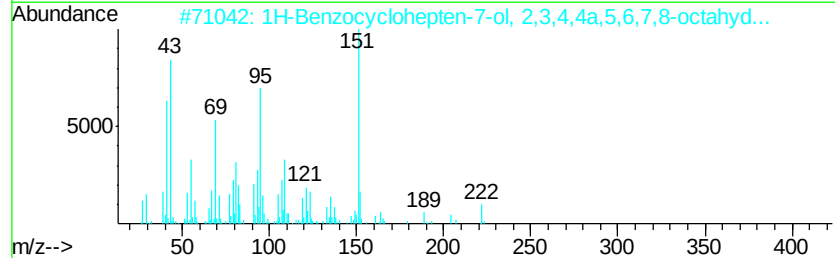
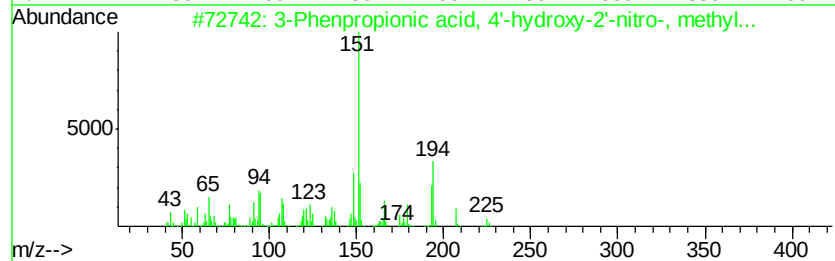
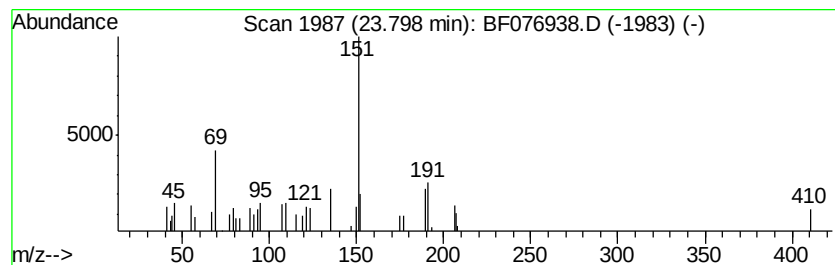
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 7 unknown23.80 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.80	3.18 ng	40656	Perylene-d12	22.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Phenpropionic acid, 4'-hydroxy...	225	C10H11N05	1000128-48-7	37
2		1H-Benzocyclohepten-7-ol, 2,3,4,...	222	C15H26O	006892-80-4	35
3		6-(3,3-Dimethyl-oxiran-2-ylidene)...	194	C12H18O2	1000187-66-2	32
4		9-Borabicyclo[3.3.1]nonan-9-amin...	151	C9H18BN	063366-66-5	27
5		2H-1,4-Benzothiazine, 3,4-dihydro-	151	C8H9NS	003080-99-7	27



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Sample : G1110-02
Misc : W
ALS Vial : 17 Sample Multiplier: 1

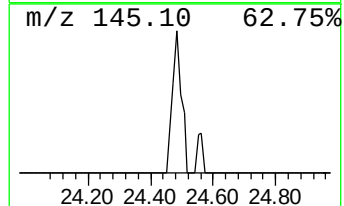
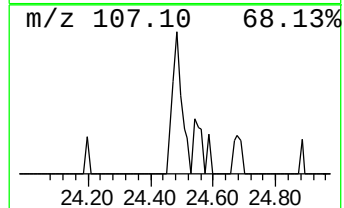
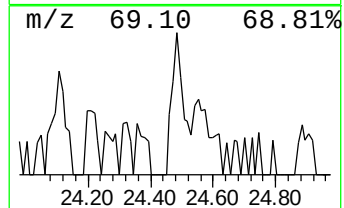
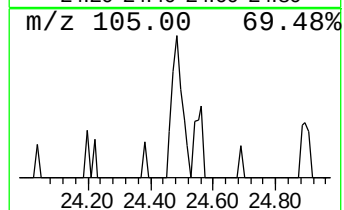
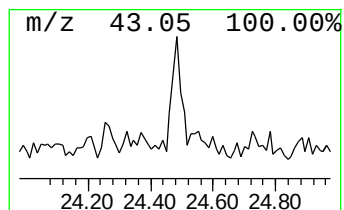
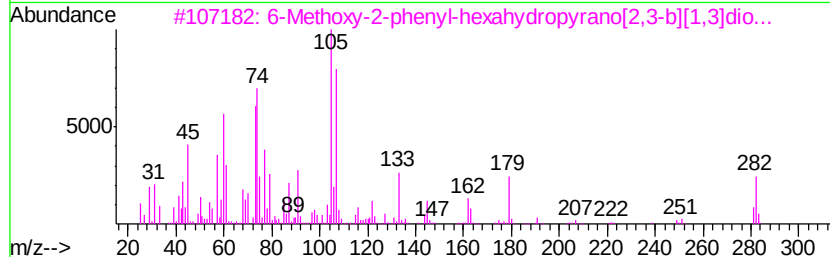
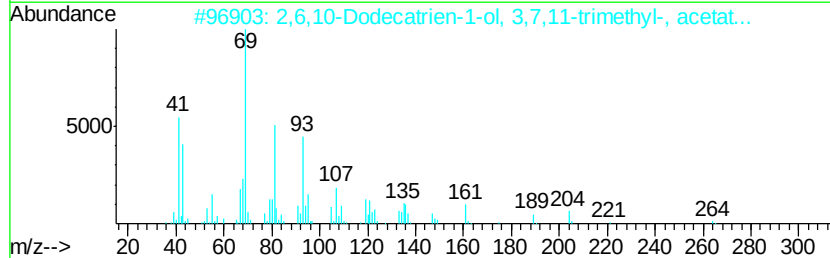
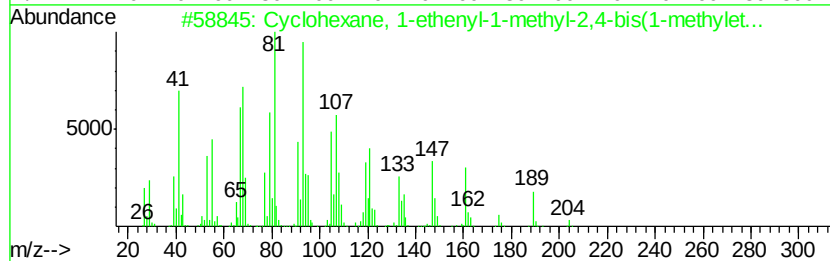
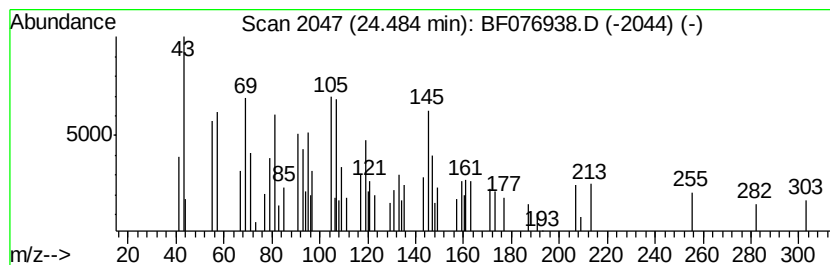
Instrument :
BNA_F
ClientSampleId :
BEM-8

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown24.48 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
24.48	5.77 ng	73753	Perylene-d12	22.92	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-ethenyl-1-methyl-...	204	C15H24	000515-13-9	32
2	2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	16
3	6-Methoxy-2-phenyl-hexahydronaphthalene...	282	C14H18O6	1000193-80-1	15
4	Cycloheptane, 4-methylene-1-meth...	204	C15H24	1000159-38-5	10
5	1,8-Nonadiene, 2,7-dimethyl-5-(1...	192	C14H24	068702-20-5	10



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011915\
Data File : BF076938.D
Acq On : 19 Jan 2015 19:59
Operator : IZ / TP
Sample : G1110-02
Misc : W
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BEM-8

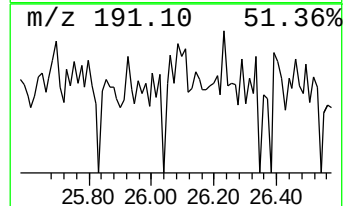
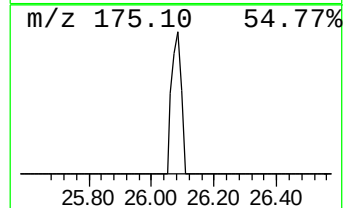
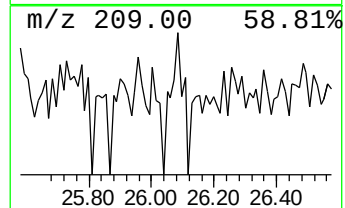
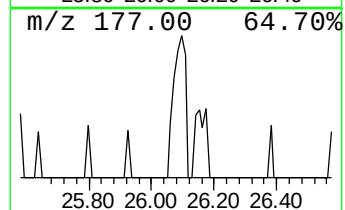
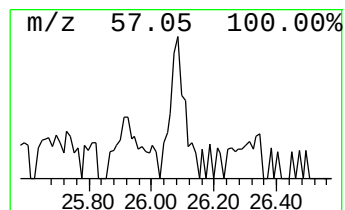
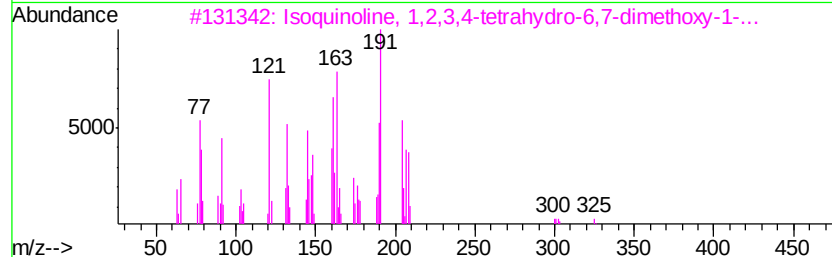
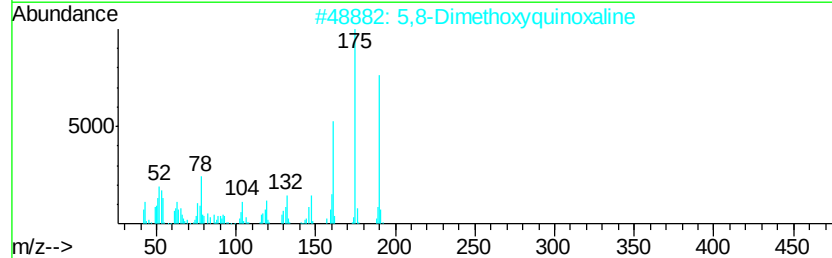
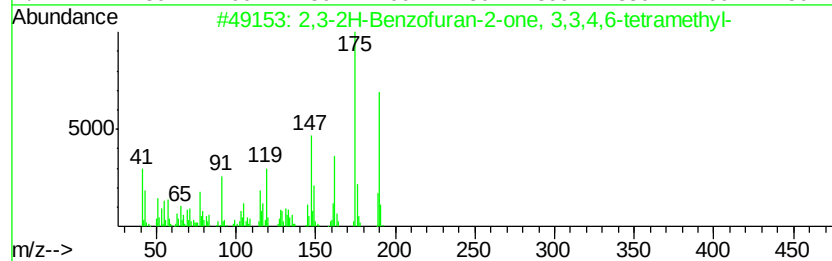
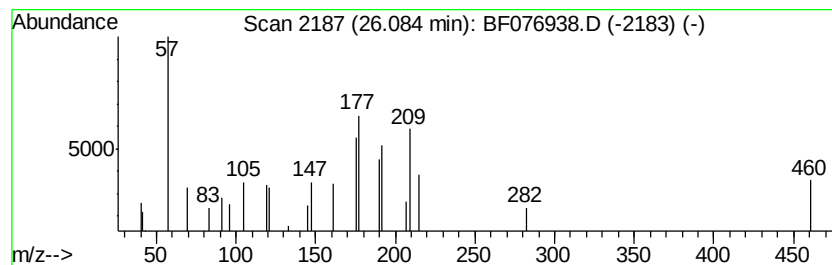
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown26.08 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.08	2.41 ng	30830	Perylene-d12	22.92

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-2H-Benzofuran-2-one, 3,3,4,6...	190	C12H14O2	086562-99-4	4	11	
2	5,8-Dimethoxyquinoxaline	190	C10H10N2O2	019506-19-5	10	10	
3	Isoquinoline, 1,2,3,4-tetrahydro...	327	C20H25N03	003423-02-7	10	10	
4	Tricyclo[6.3.0.0(1,5)]undec-2-en...	190	C13H18O	1000153-99-7	9	9	
5	Benzenemethanol, 3,4-dichloro-.a...	190	C8H8Cl2O	001475-11-2	9	9	



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011915\
Data File : BF076938.D
Acq On : 19 Jan 2015 19:59
Operator : IZ / TP
Sample : G1110-02
Misc : W
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BEM-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.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...	4.10	18.6	ng	166738	1	7.97	178895	20.0
unknown7.46	7.46	78.0	ng	697209	1	7.97	178895	20.0
unknown15.92	15.92	2.4	ng	30762	3	15.01	259650	20.0
Squalene	22.47	3.4	ng	43977	6	22.92	255733	20.0
unknown23.80	23.80	3.2	ng	40656	6	22.92	255733	20.0
unknown24.48	24.48	5.8	ng	73753	6	22.92	255733	20.0
unknown26.08	26.08	2.4	ng	30830	6	22.92	255733	20.0