

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121315\
 Data File : BF083767.D
 Acq On : 14 Dec 2015 9:17
 Operator : UM/IZ
 Sample : G4648-15
 Misc :
 ALS Vial : 57 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-09-(0-0.16)

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-BF121315.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	2.224	10	12	26	rVB2	27697	83222	3.12%	0.321%
2	3.687	137	140	145	rVB	18493	31501	1.18%	0.121%
3	5.116	262	265	268	rBV	423358	558926	20.92%	2.154%
4	5.527	298	301	304	rBV	2370551	2416077	90.44%	9.312%
5	6.544	387	390	393	rBV	2143989	2336670	87.47%	9.006%
6	6.682	400	402	405	rBV	1970981	2671458	100.00%	10.296%
7	6.922	420	423	425	rBV	665249	641028	24.00%	2.471%
8	7.082	434	437	439	rVB	1441585	1925895	72.09%	7.422%
9	7.482	469	472	474	rBV	1487794	1787393	66.91%	6.889%
10	7.562	477	479	482	rBV	27001	34123	1.28%	0.132%
11	7.927	508	511	512	rBV	23596	28710	1.07%	0.111%
12	8.099	524	526	528	rBV3	28187	30254	1.13%	0.117%
13	8.202	533	535	537	rBV	985238	827730	30.98%	3.190%
14	8.533	561	564	567	rBV	31998	37049	1.39%	0.143%
15	8.625	570	572	575	rVB	29965	33070	1.24%	0.127%
16	9.276	626	629	632	rBV	2592911	2367408	88.62%	9.124%
17	9.402	638	640	643	rVB	41367	47758	1.79%	0.184%
18	9.665	661	663	666	rBV	538634	564030	21.11%	2.174%
19	9.893	682	683	686	rVB2	45415	33710	1.26%	0.130%
20	9.950	686	688	691	rBV	738165	836299	31.30%	3.223%
21	10.373	723	725	726	rBV	27943	47772	1.79%	0.184%
22	10.396	726	727	728	rVB	66454	45869	1.72%	0.177%
23	10.613	744	746	749	rBV	29342	40091	1.50%	0.155%
24	10.739	754	757	759	rBV	1640728	1573322	58.89%	6.064%
25	10.865	766	768	772	rVB2	81125	92946	3.48%	0.358%
26	10.956	774	776	778	rVB2	36017	40836	1.53%	0.157%
27	11.059	783	785	787	rBV2	19804	31167	1.17%	0.120%
28	11.139	790	792	795	rBV	36101	33267	1.25%	0.128%
29	11.311	804	807	809	rBV	58662	57928	2.17%	0.223%
30	11.436	816	818	820	rBV	903102	827900	30.99%	3.191%
31	11.962	863	864	866	rBV	43997	40732	1.52%	0.157%
32	12.145	876	880	882	rBV2	21027	37204	1.39%	0.143%
33	12.271	885	891	894	rBV	15447	28973	1.08%	0.112%
34	12.419	902	904	908	rBV3	14551	31193	1.17%	0.120%

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35	12.476	908	909	911	rBV	41765	41372	1.55%	0.159%
36	12.636	922	923	925	rBV2	40674	50311	1.88%	0.194%
37	12.671	925	926	931	rVB	32334	39281	1.47%	0.151%
38	12.796	932	937	938	rBV2	17557	36445	1.36%	0.140%
39	12.819	938	939	940	rVV	24997	28713	1.07%	0.111%
40	12.842	940	941	945	rVV2	139325	190392	7.13%	0.734%
41	12.922	947	948	949	rVB	67706	47321	1.77%	0.182%
42	13.014	954	956	958	rVV	1825671	1748491	65.45%	6.739%
43	13.174	968	970	973	rBV2	43362	78161	2.93%	0.301%
44	13.368	985	987	990	rVV3	27722	46006	1.72%	0.177%
45	13.425	990	992	995	rVV3	12427	32500	1.22%	0.125%
46	13.505	996	999	1001	rVV	73510	110836	4.15%	0.427%
47	13.551	1001	1003	1005	rVV	221544	219600	8.22%	0.846%
48	13.597	1005	1007	1010	rVV2	57063	104783	3.92%	0.404%
49	13.642	1010	1011	1013	rVV2	77230	103161	3.86%	0.398%
50	13.677	1013	1014	1015	rVV	131498	103744	3.88%	0.400%
51	13.722	1015	1018	1021	rVB2	52535	89240	3.34%	0.344%
52	13.871	1029	1031	1033	rVB	60270	72548	2.72%	0.280%
53	13.917	1033	1035	1038	rBV3	84402	142685	5.34%	0.550%
54	13.985	1038	1041	1043	rBV	112779	147267	5.51%	0.568%
55	14.065	1043	1048	1050	rBV	727417	883042	33.05%	3.403%
56	14.237	1061	1063	1065	rBV	57396	59558	2.23%	0.230%
57	14.294	1066	1068	1069	rVV	72910	71212	2.67%	0.274%
58	14.339	1069	1072	1074	rVV2	31385	54908	2.06%	0.212%
59	14.419	1078	1079	1081	rVB2	29225	36272	1.36%	0.140%
60	14.545	1088	1090	1092	rBV	64206	72246	2.70%	0.278%
61	14.591	1092	1094	1096	rVB	71002	69389	2.60%	0.267%
62	14.739	1103	1107	1109	rBV2	76873	121159	4.54%	0.467%
63	14.785	1109	1111	1114	rVV	34755	51384	1.92%	0.198%
64	14.842	1114	1116	1120	rVB	47062	62248	2.33%	0.240%
65	15.060	1132	1135	1136	rBV	21316	35157	1.32%	0.135%
66	15.174	1143	1145	1150	rVB2	41342	69287	2.59%	0.267%
67	15.505	1171	1174	1176	rBV	408042	563322	21.09%	2.171%
68	15.551	1176	1178	1185	rVB	36680	77192	2.89%	0.298%
69	15.985	1213	1216	1218	rBV	24523	37918	1.42%	0.146%
70	16.763	1282	1284	1289	rVB6	13477	28094	1.05%	0.108%

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Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

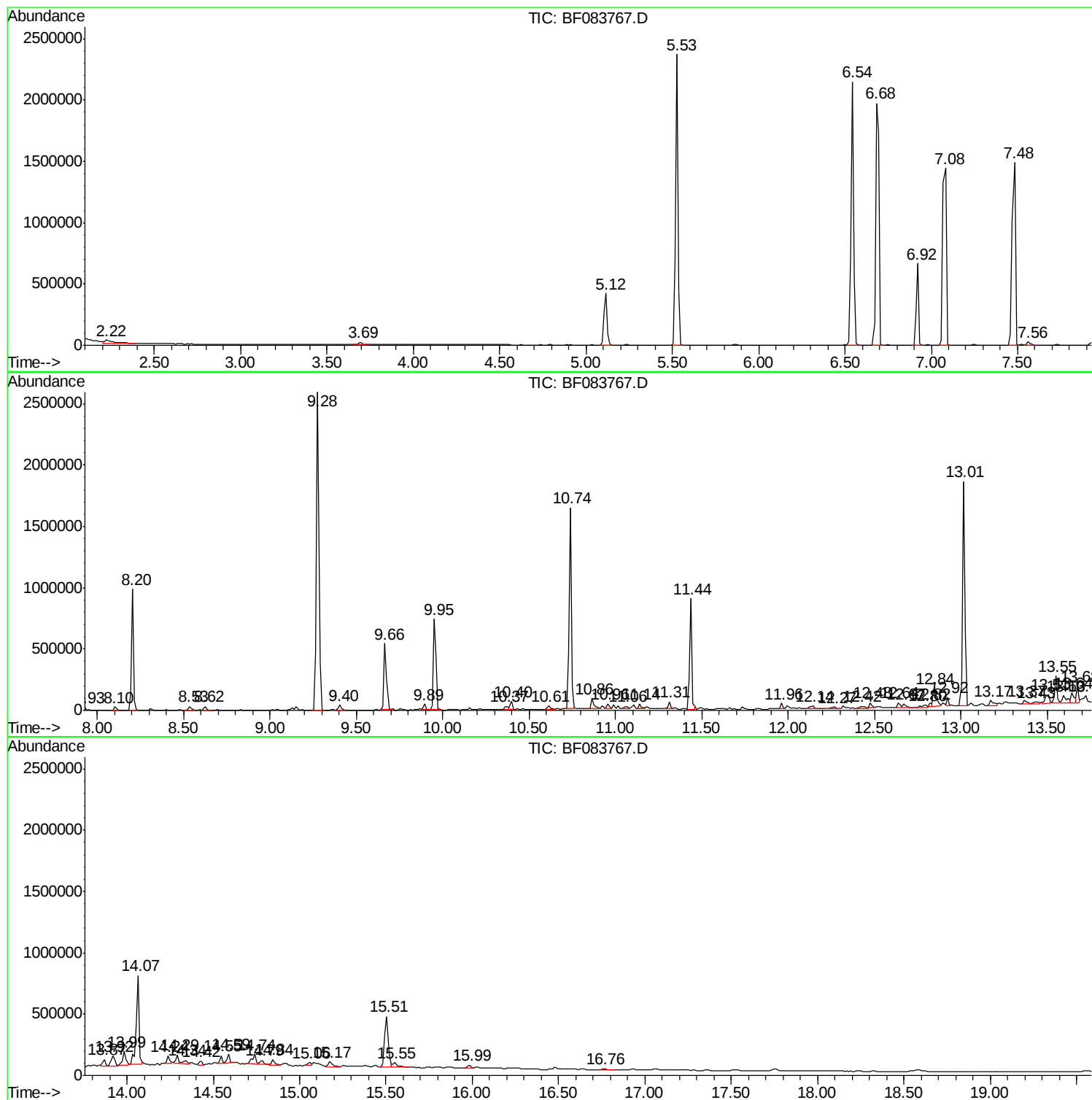
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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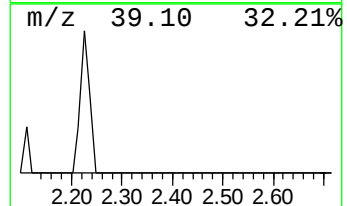
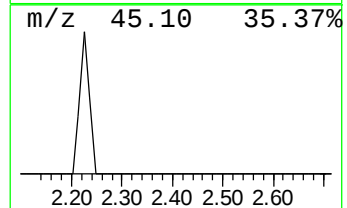
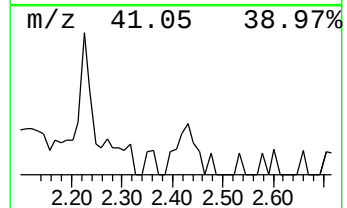
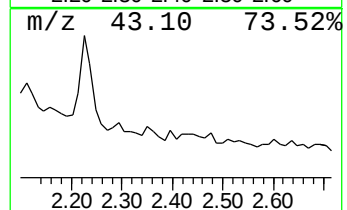
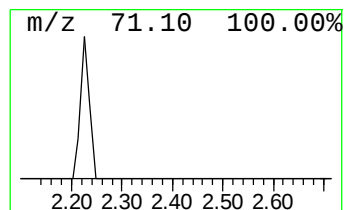
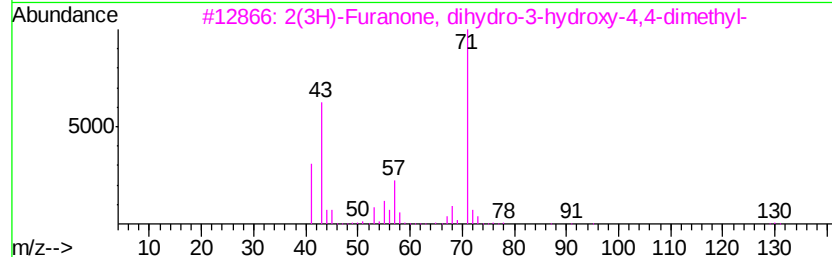
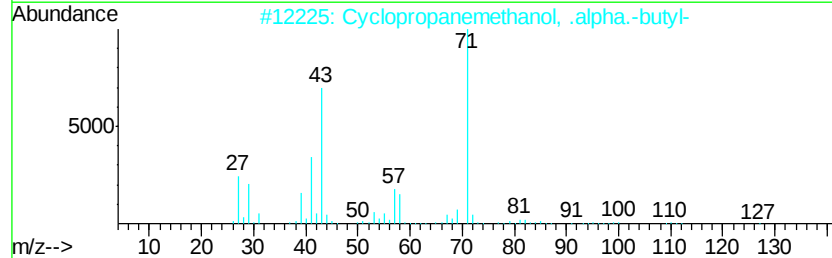
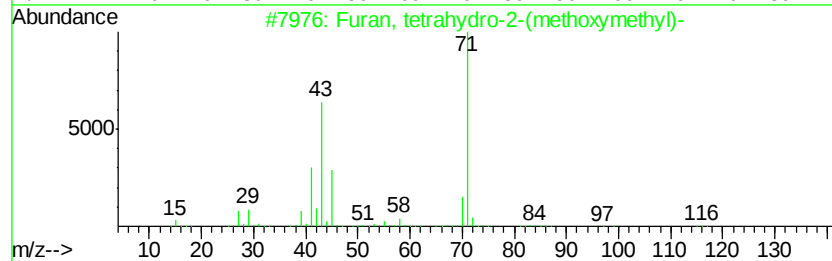
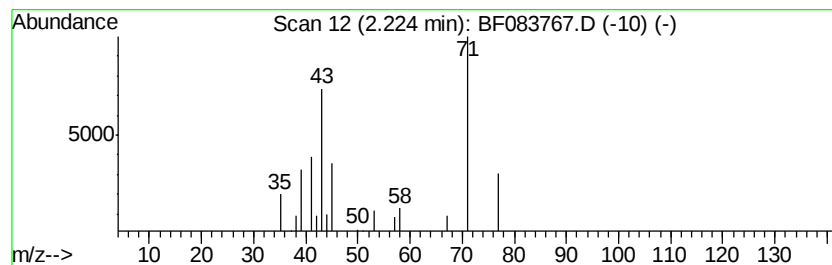
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown2.22 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.22	2.60 ng	83222	1,4-Dichlorobenzene-d4	6.92

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Furan, tetrahydro-2-(methoxymeth...	116	C6H12O2	019354-27-9	23
2			Cyclopropanemethanol, .alpha.-bu...	128	C8H16O	004379-16-2	17
3			2(3H)-Furanone, dihydro-3-hydrox...	130	C6H10O3	052126-90-6	9
4			Pantolactone	130	C6H10O3	000599-04-2	9
5			3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	9



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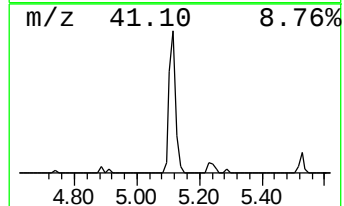
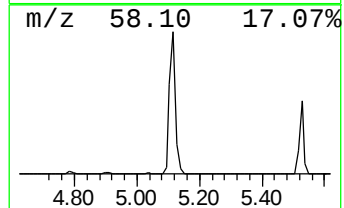
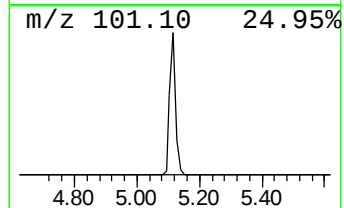
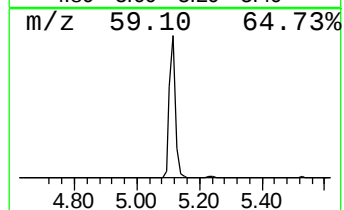
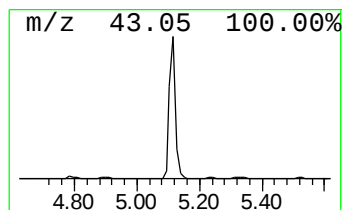
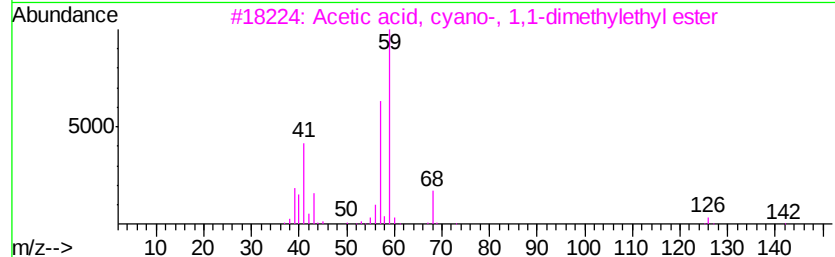
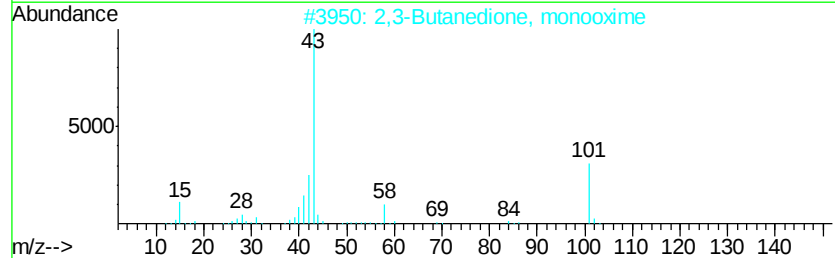
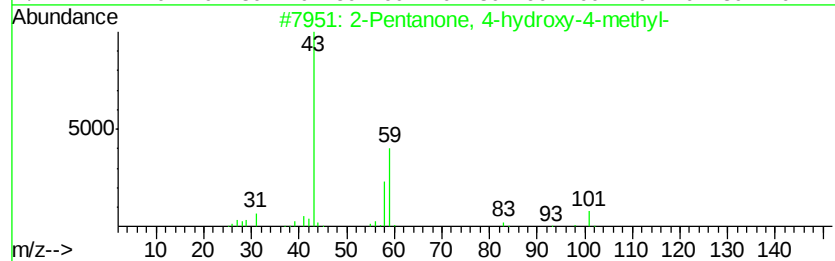
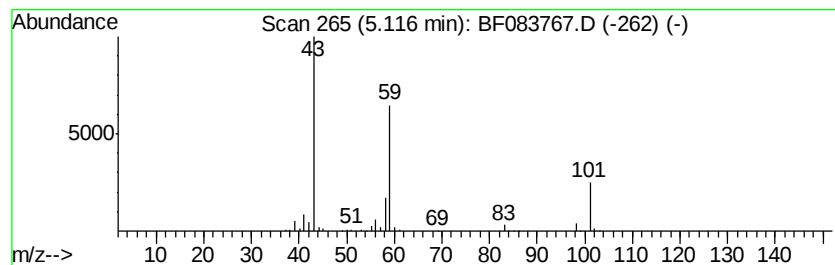
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	17.44 ng	558926	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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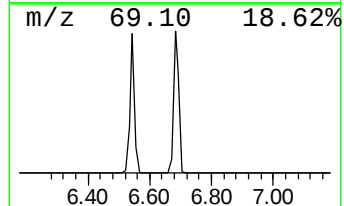
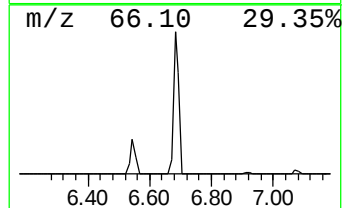
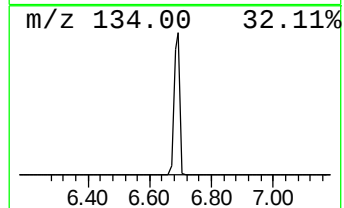
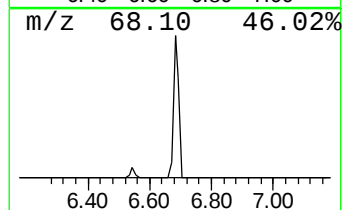
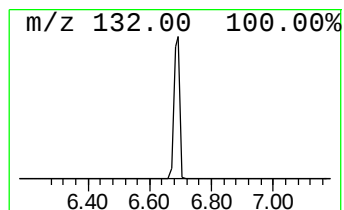
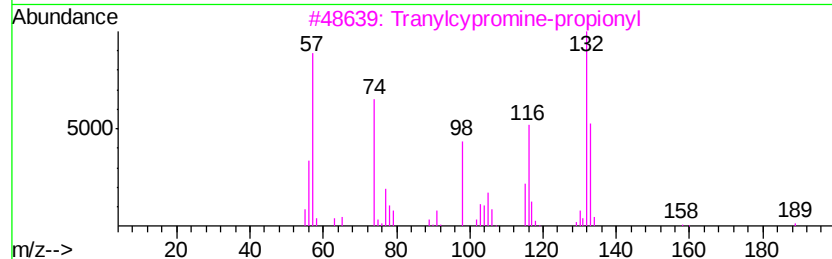
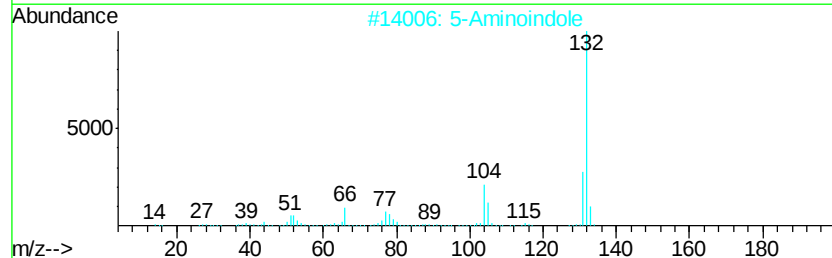
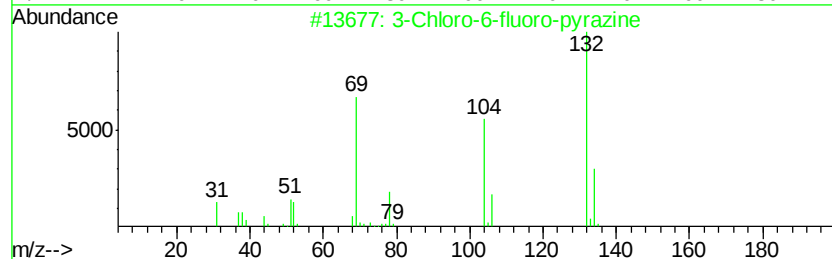
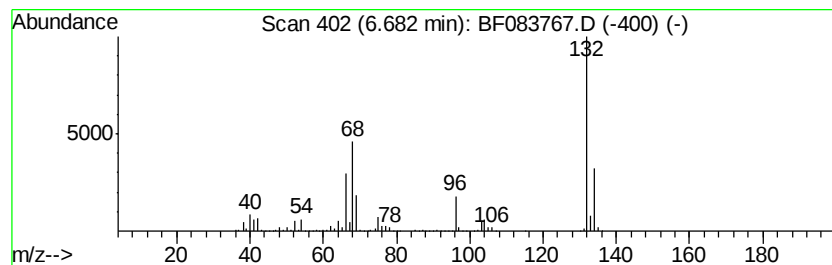
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	83.35 ng	2671460	1,4-Dichlorobenzene-d4	6.92

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			Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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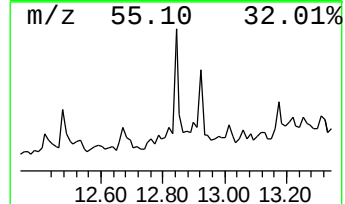
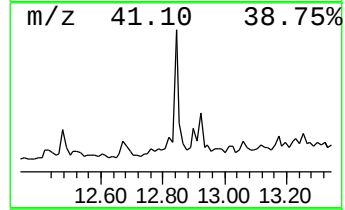
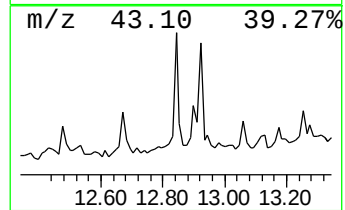
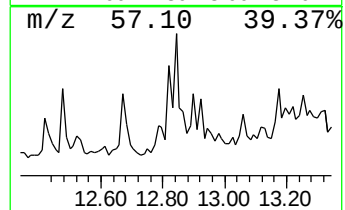
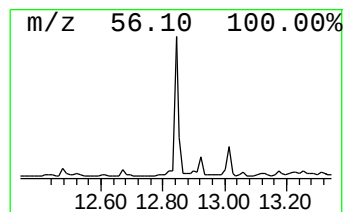
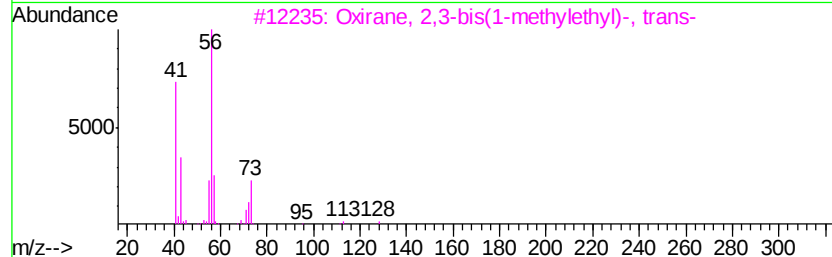
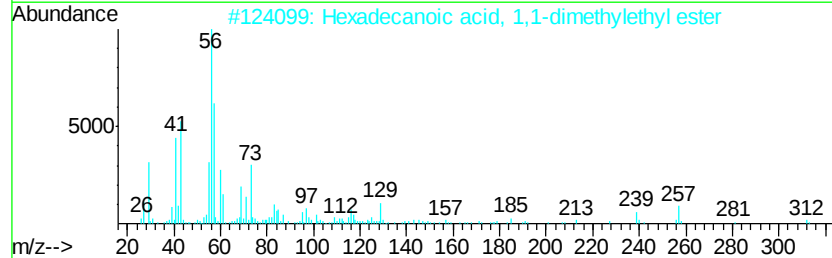
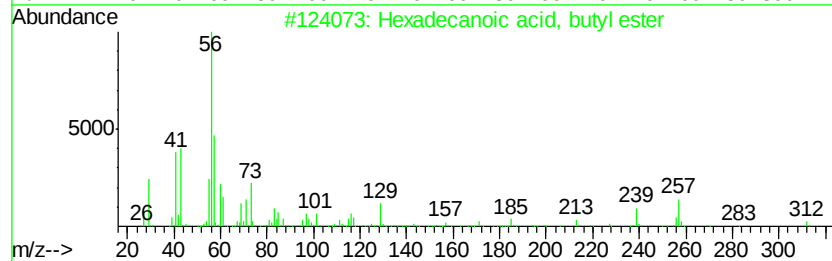
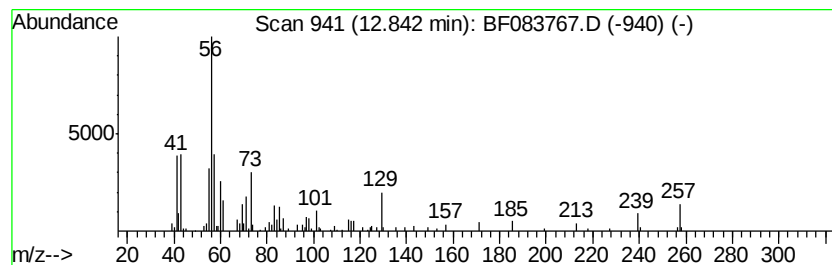
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.84	4.31 ng	190392	Chrysene-d12	14.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	90
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	86
3		Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	38
4		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	32
5		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083767.D
Acq On : 14 Dec 2015 9:17
Operator : UM/IZ
Sample : G4648-15
Misc :
ALS Vial : 57 Sample Multiplier: 1

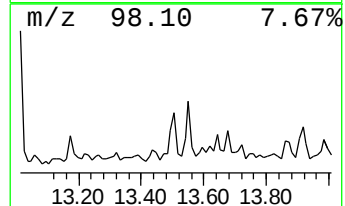
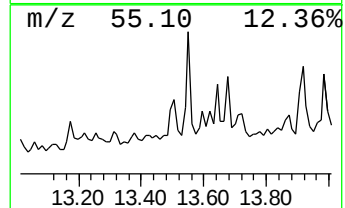
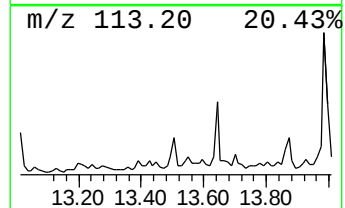
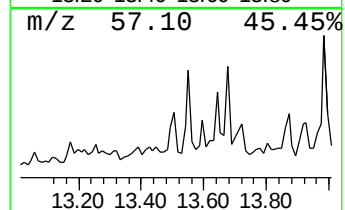
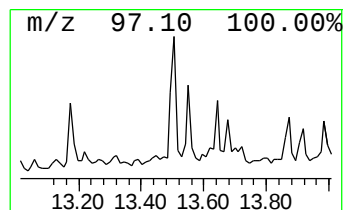
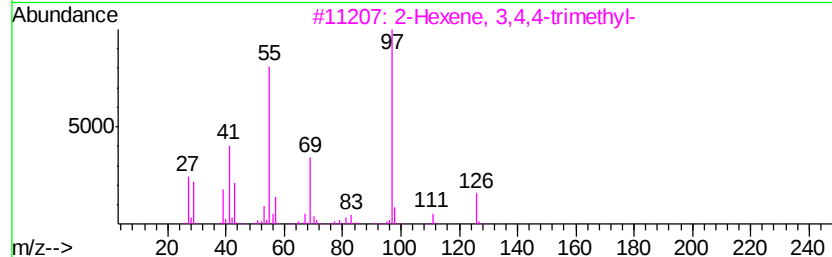
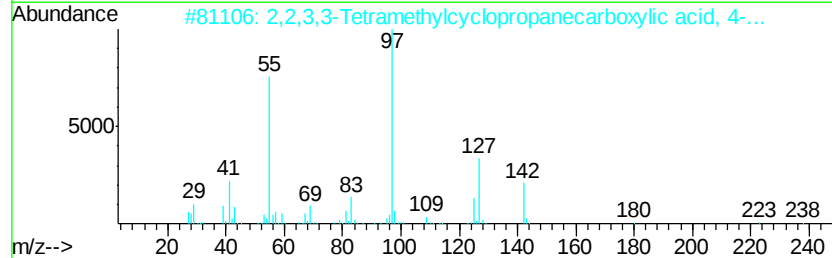
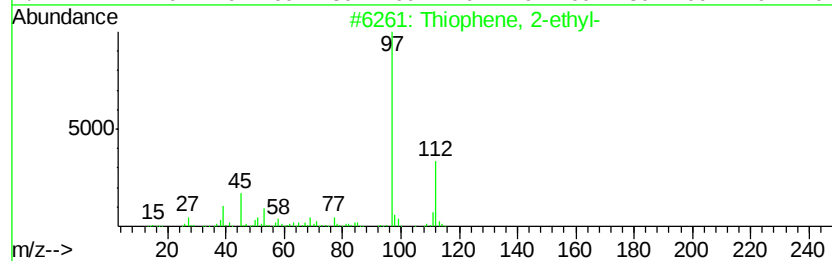
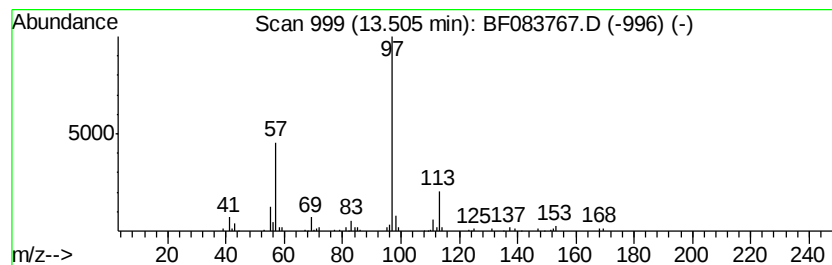
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ClientSampleId :
SB-09-(0-0.16)

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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 Thiophene, 2-ethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.51	2.51 ng	110836	Chrysene-d12	14.07	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophene, 2-ethyl-	112	C6H8S	000872-55-9	53
2	2,2,3,3-Tetramethylcyclopropanec...	238	C15H26O2	1000221-97-5	50
3	2-Hexene, 3,4,4-trimethyl-	126	C9H18	053941-19-8	45
4	4-Methyl-2,3-hexadien-1-ol	112	C7H12O	1000196-09-6	40
5	2H-Pyran-2-one, 5,6-dihydro-6-pe...	168	C10H16O2	054814-64-1	40



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083767.D
Acq On : 14 Dec 2015 9:17
Operator : UM/IZ
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ClientSampleId :
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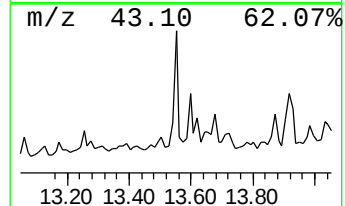
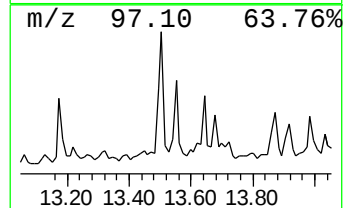
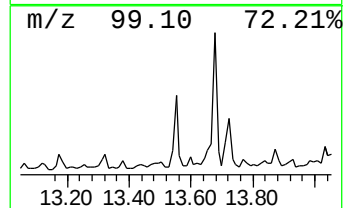
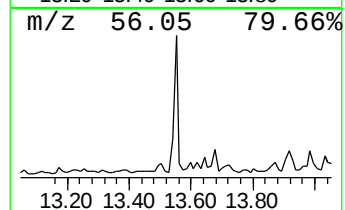
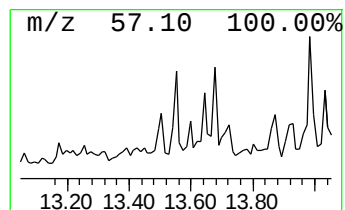
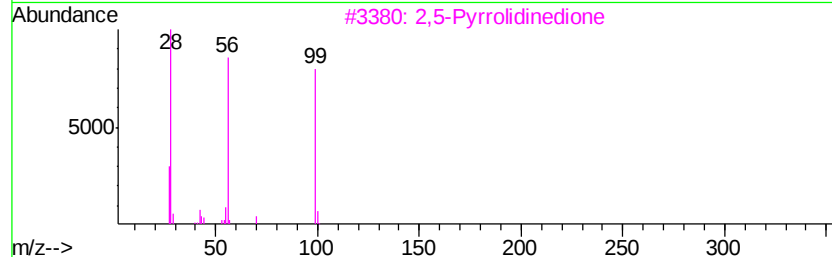
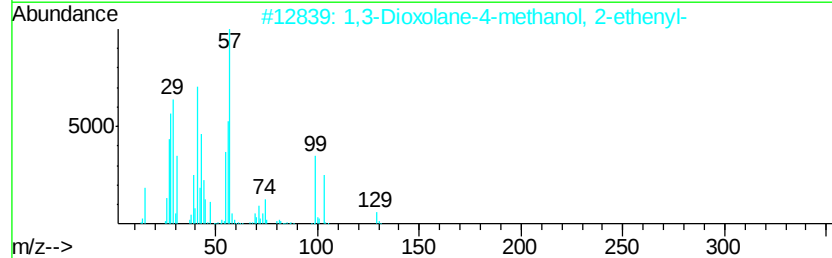
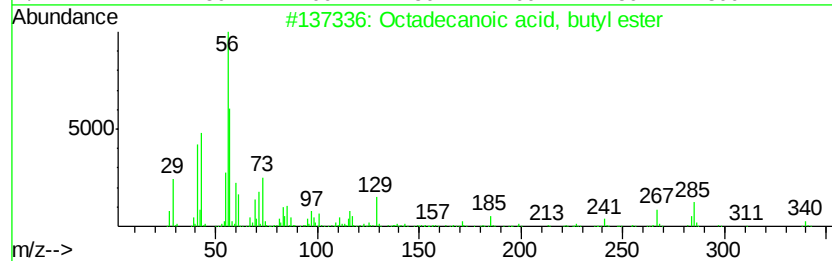
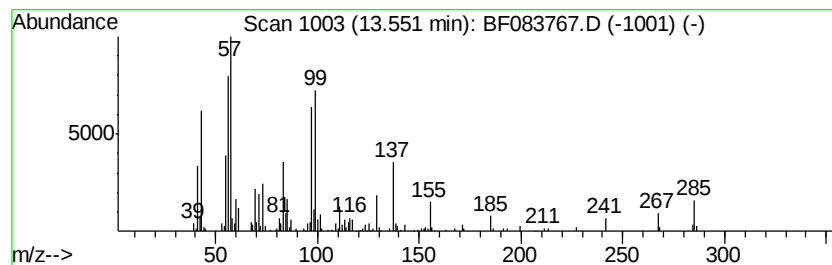
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown13.55 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.55	4.97 ng	219600	Chrysene-d12	14.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	43
2		1,3-Dioxolane-4-methanol, 2-ethenyl-	130	C6H10O3	004313-32-0	38
3		2,5-Pyrrolidinedione	99	C4H5NO2	000123-56-8	35
4		Acetamide, N-ethenyl-N-methyl-	99	C5H9NO	003195-78-6	35
5		n-Capric acid isobutyl ester	228	C14H28O2	030673-38-2	27



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083767.D
Acq On : 14 Dec 2015 9:17
Operator : UM/IZ
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Misc :
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Instrument :
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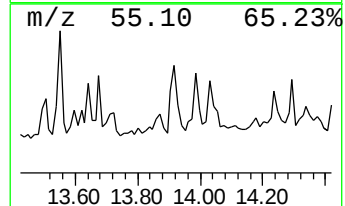
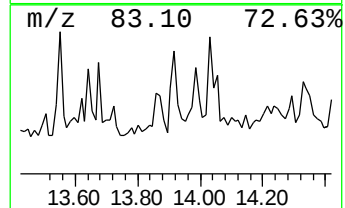
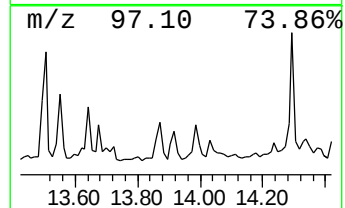
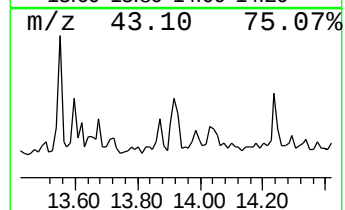
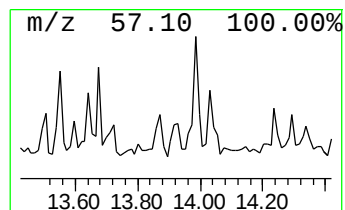
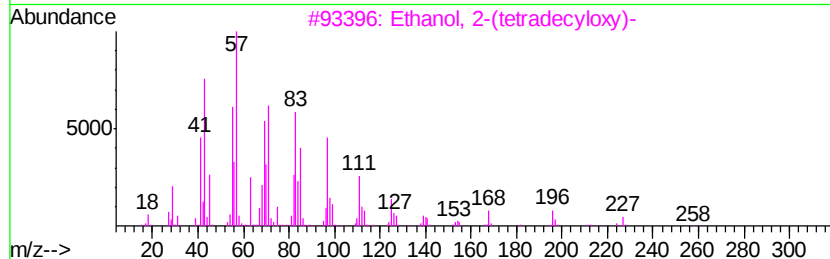
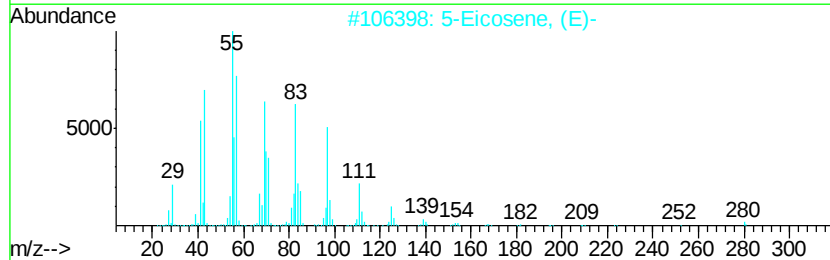
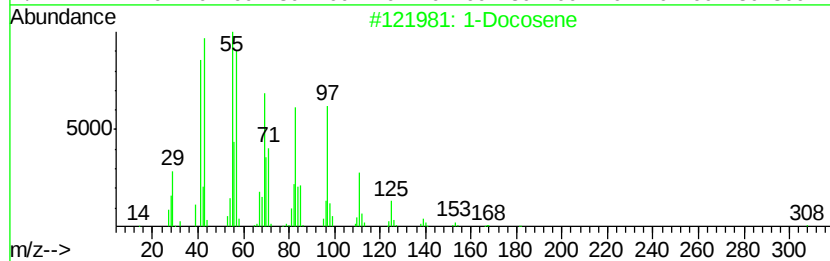
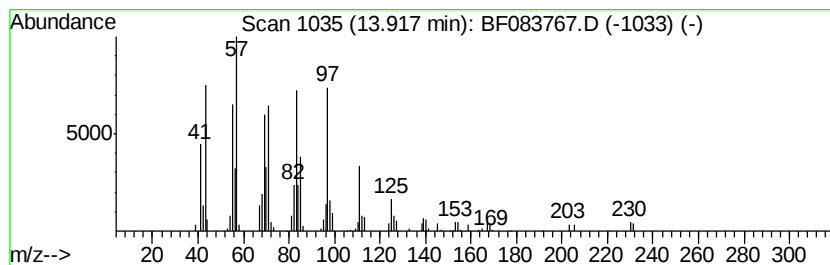
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Docosene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.92	3.23 ng	142685	Chrysene-d12	14.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Docosene	308	C22H44	001599-67-3	74
2		5-Eicosene, (E)-	280	C20H40	074685-30-6	68
3		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	68
4		1-Nonadecene	266	C19H38	018435-45-5	68
5		1-Octadecanol	270	C18H38O	000112-92-5	60



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
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Acq On : 14 Dec 2015 9:17
Operator : UM/IZ
Sample : G4648-15
Misc :
ALS Vial : 57 Sample Multiplier: 1

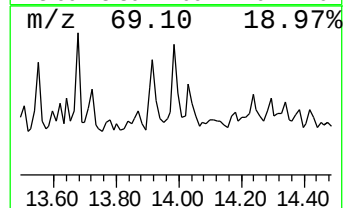
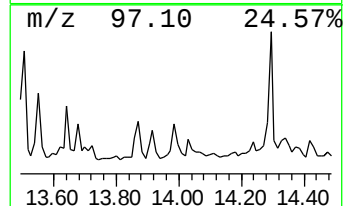
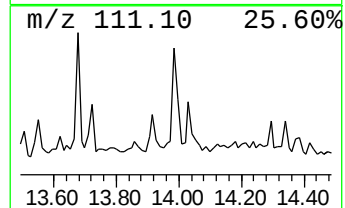
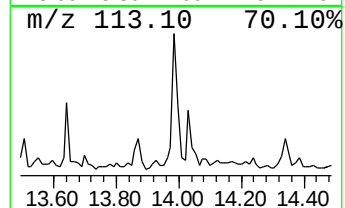
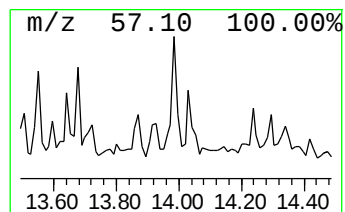
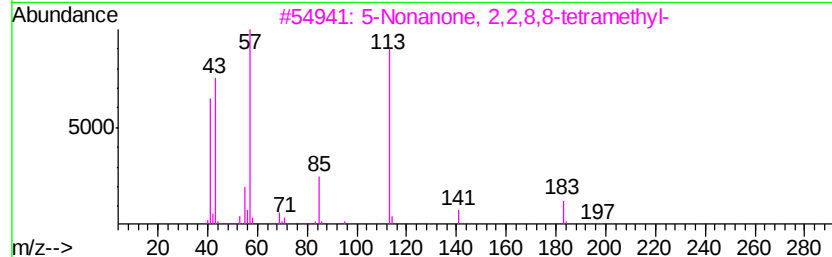
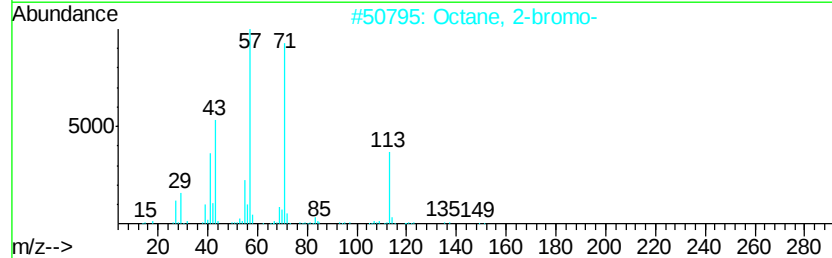
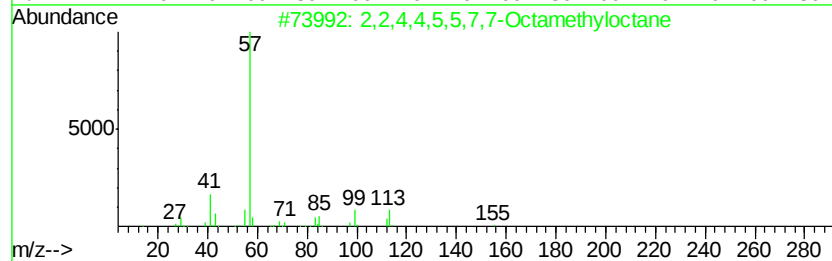
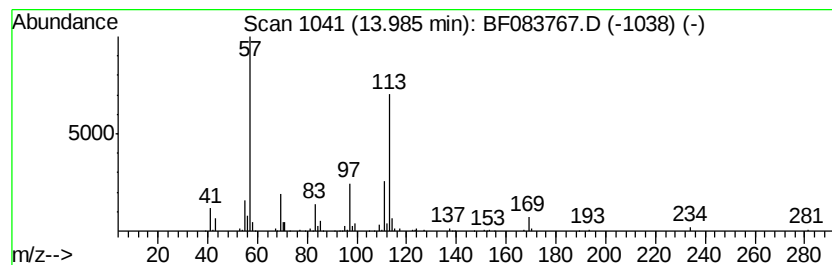
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown13.99 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.99	3.34 ng	147267	Chrysene-d12	14.07	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2,4,4,5,5,7,7-Octamethyloctane	226	C16H34	005171-85-7	37
2	Octane, 2-bromo-	192	C8H17Br	000557-35-7	37
3	5-Nonanone, 2,2,8,8-tetramethyl-	198	C13H26O	005709-95-5	32
4	4-Fluoro-6-aminopyrimidine	113	C4H4FN3	051421-96-6	27
5	1H-Azepin-1-amine, hexahydro-N-(...	168	C10H20N2	028075-23-2	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121315\
Data File : BF083767.D
Acq On : 14 Dec 2015 9:17
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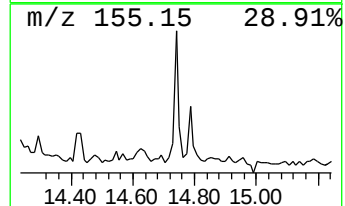
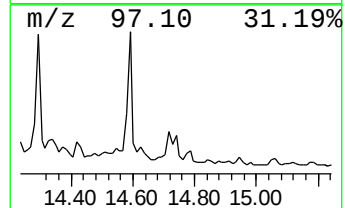
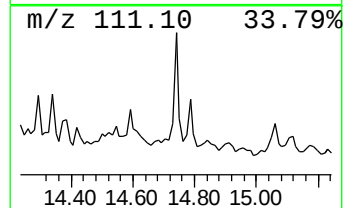
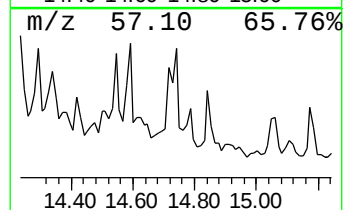
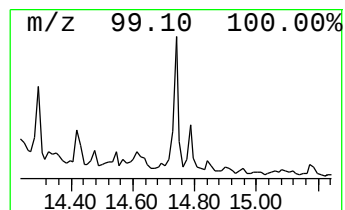
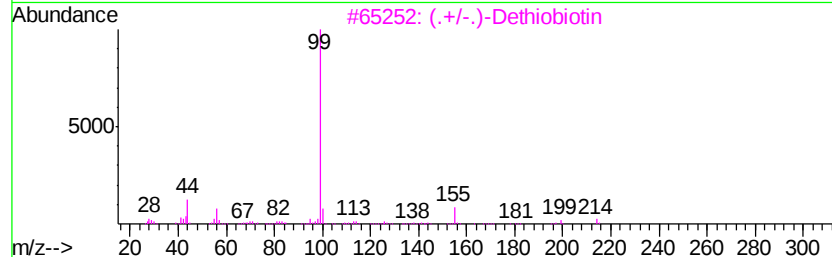
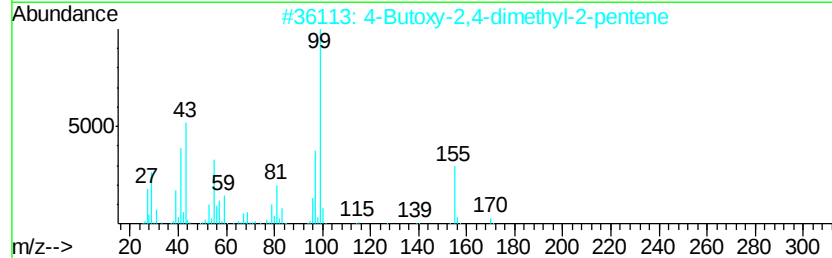
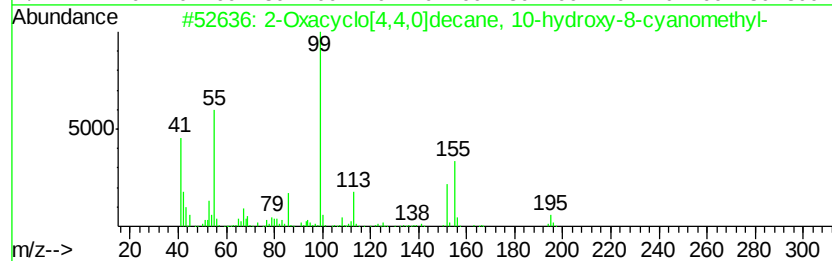
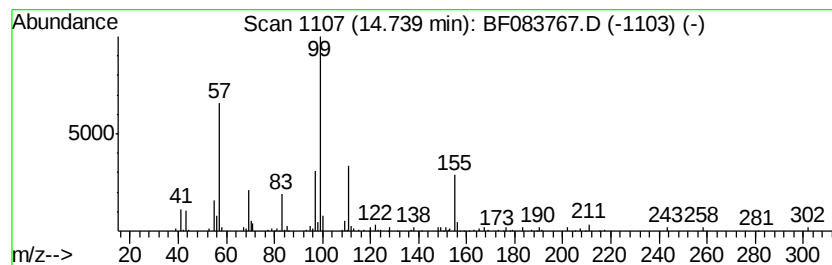
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown14.74 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.74	2.74 ng	121159	Chrysene-d12	14.07

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Oxacyclo[4,4,0]decane, 10-hydr...	195	C11H17N02	1000130-46-5	40		
2	4-Butoxy-2,4-dimethyl-2-pentene	170	C11H22O	1000159-08-7	39		
3	(.+/-)-Dethiobiotin	214	C10H18N2O3	000636-20-4	38		
4	1,3,2-Dioxaborolane, 2,4-diethyl-	128	C6H13B02	057633-63-3	38		
5	1-Pyrrolidinocarbonylmethyl pipe...	197	C10H19N3O	039890-45-4	36		



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121315\
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Acq On : 14 Dec 2015 9:17
Operator : UM/IZ
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Misc :
ALS Vial : 57 Sample Multiplier: 1

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

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

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					#	RT	Resp	Conc
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2-Pentanone, 4-hy...	5.12	17.4	ng	558926	1	6.92	641028	20.0
unknown6.68	6.68	83.3	ng	2671460	1	6.92	641028	20.0
Hexadecanoic acid...	12.84	4.3	ng	190392	5	14.07	883042	20.0
Thiophene, 2-ethyl-	13.51	2.5	ng	110836	5	14.07	883042	20.0
unknown13.55	13.55	5.0	ng	219600	5	14.07	883042	20.0
1-Docosene	13.92	3.2	ng	142685	5	14.07	883042	20.0
unknown13.99	13.99	3.3	ng	147267	5	14.07	883042	20.0
unknown14.74	14.74	2.7	ng	121159	5	14.07	883042	20.0