

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG061115\
 Data File : BG017626.D
 Acq On : 12 Jun 2015 1:08
 Operator : TP/IZ
 Sample : G2523-12
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PZ-6-6-4-15

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_G\METHODS\8270-BG060315.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	4.629	325	330	336	rBV2	20832	32559	1.04%	0.281%
2	5.117	408	413	424	rBV	235651	345154	10.97%	2.975%
3	6.738	683	689	699	rBV	165232	251420	7.99%	2.167%
4	7.067	735	745	753	rBV	456027	715590	22.75%	6.168%
5	7.531	817	824	831	rBV	97763	157655	5.01%	1.359%
6	7.849	871	878	885	rVB	417847	633911	20.15%	5.464%
7	8.695	1015	1022	1029	rBV	361432	580108	18.44%	5.000%
8	10.322	1292	1299	1311	rBV	122572	219996	6.99%	1.896%
9	12.620	1685	1690	1696	rBV8	18377	36733	1.17%	0.317%
10	12.819	1718	1724	1730	rBV	1043561	1448371	46.04%	12.484%
11	13.472	1830	1835	1841	rBV8	23900	41231	1.31%	0.355%
12	13.824	1889	1895	1898	rBV8	14586	32895	1.05%	0.284%
13	14.206	1955	1960	1967	rVB2	238442	356900	11.35%	3.076%
14	14.341	1978	1983	1986	rBV7	25489	36047	1.15%	0.311%
15	14.511	2006	2012	2015	rBV8	19698	32777	1.04%	0.283%
16	15.275	2139	2142	2146	rBV5	28885	36224	1.15%	0.312%
17	15.710	2208	2216	2222	rBV	1137560	1570409	49.92%	13.535%
18	15.910	2244	2250	2255	rBV8	37634	66769	2.12%	0.575%
19	16.962	2423	2429	2434	rBV	333248	473848	15.06%	4.084%
20	17.872	2580	2584	2591	rBV6	55119	77734	2.47%	0.670%
21	19.159	2800	2803	2807	rBV5	34946	47905	1.52%	0.413%
22	19.605	2873	2879	2884	rBV	2745522	3145759	100.00%	27.114%
23	20.487	3025	3029	3033	rBV	110301	133094	4.23%	1.147%
24	20.875	3092	3095	3100	rBV6	29022	36685	1.17%	0.316%
25	21.157	3138	3143	3149	rBV	469079	574766	18.27%	4.954%
26	23.354	3510	3517	3527	rVB2	266150	517610	16.45%	4.461%

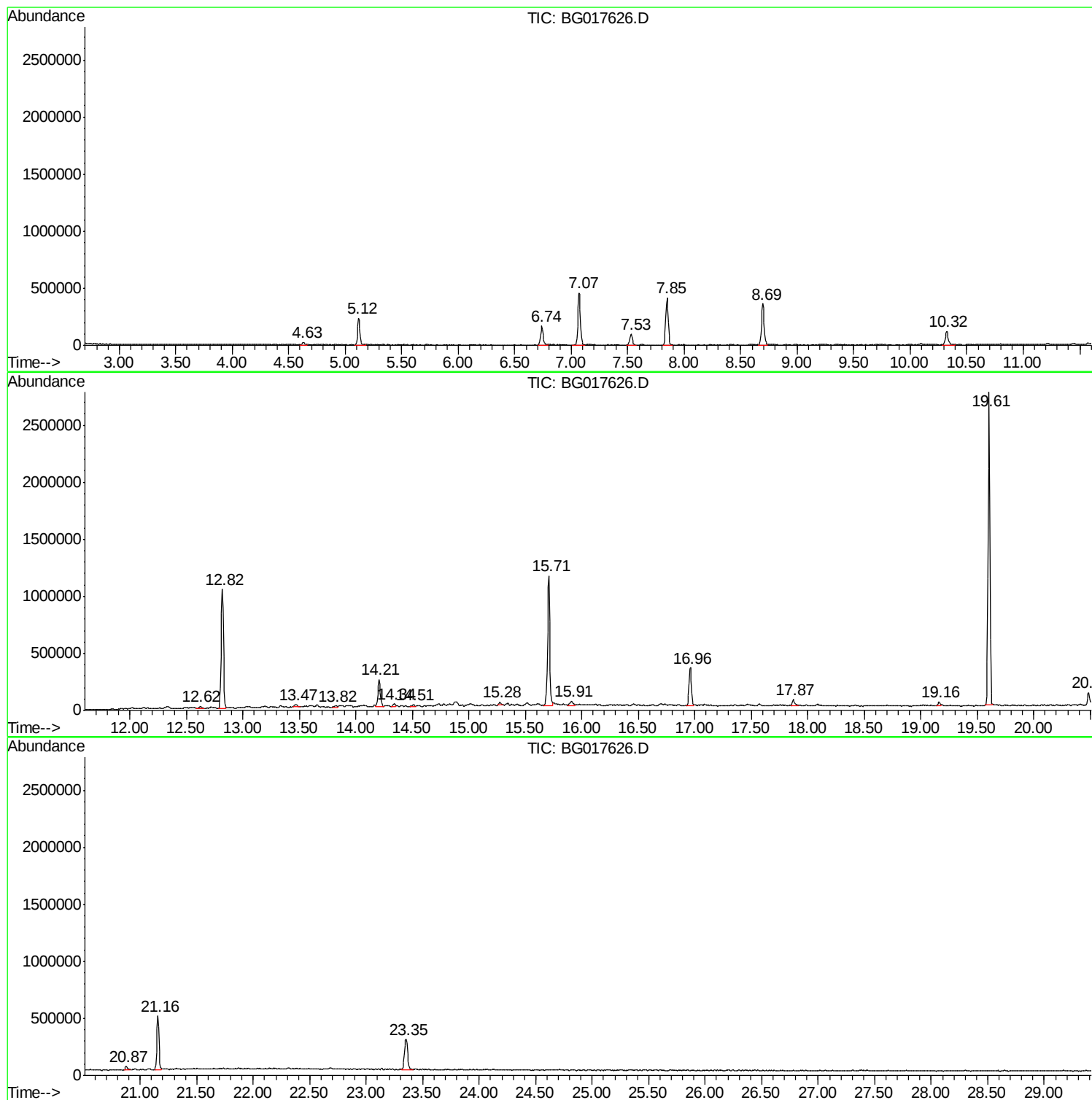
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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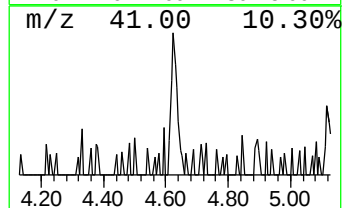
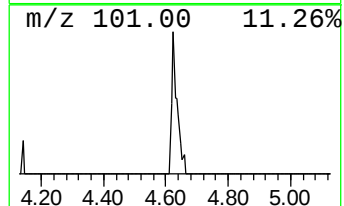
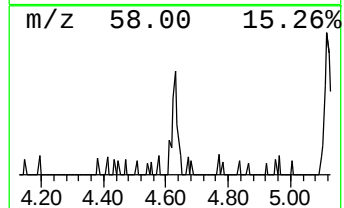
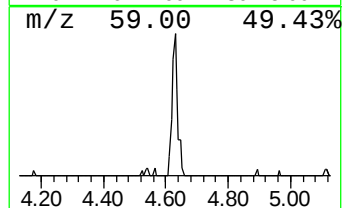
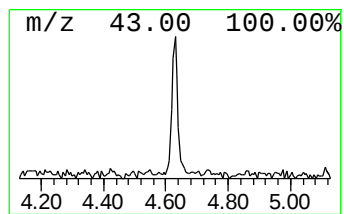
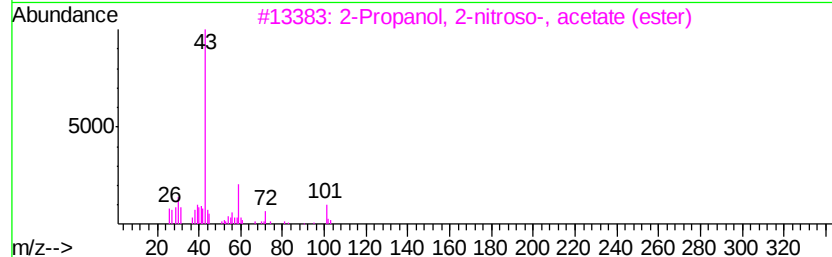
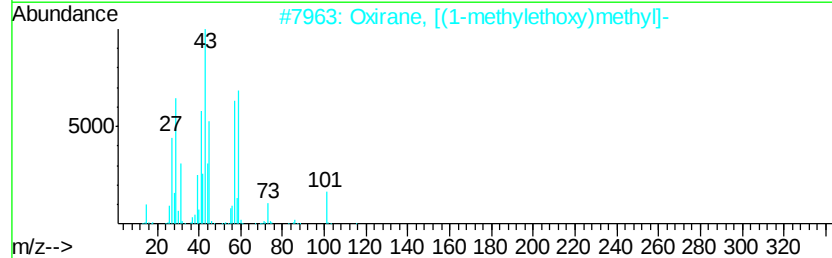
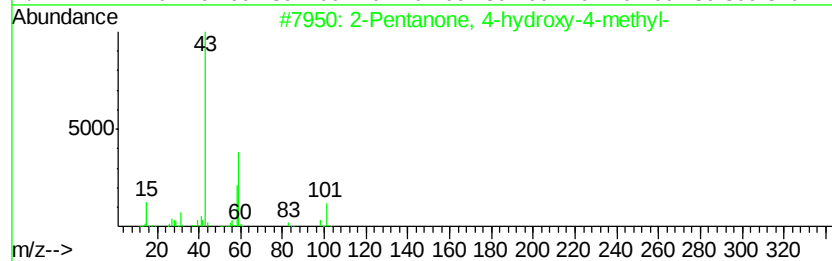
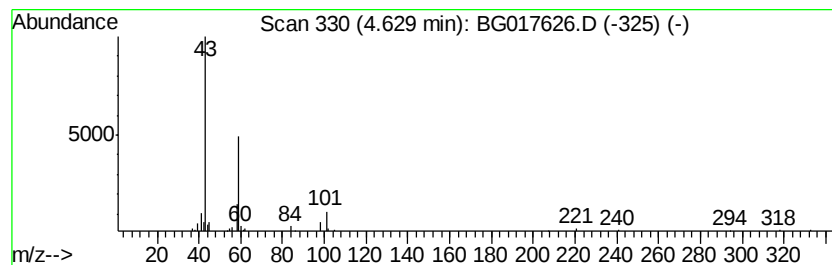
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.63	4.13 ng	32559	1,4-Dichlorobenzene-d4	7.53

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2			Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	36
3			2-Propanol, 2-nitroso-, acetate ...	131	C5H9NO3	006931-04-0	33
4			Formamide, N-butyl-	101	C5H11NO	000871-71-6	9
5			Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	9



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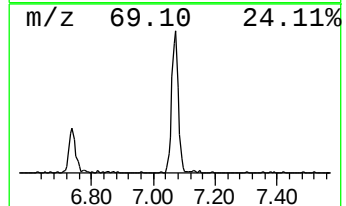
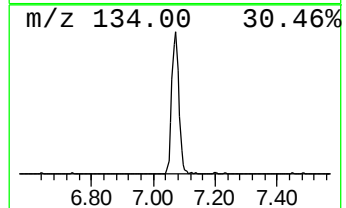
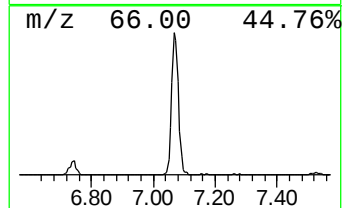
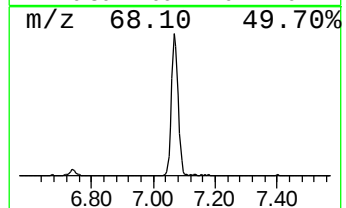
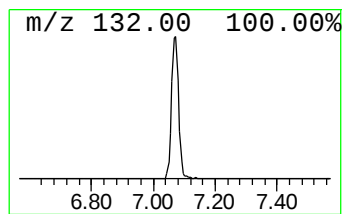
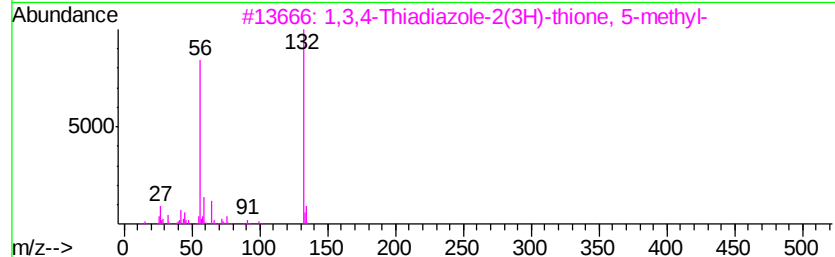
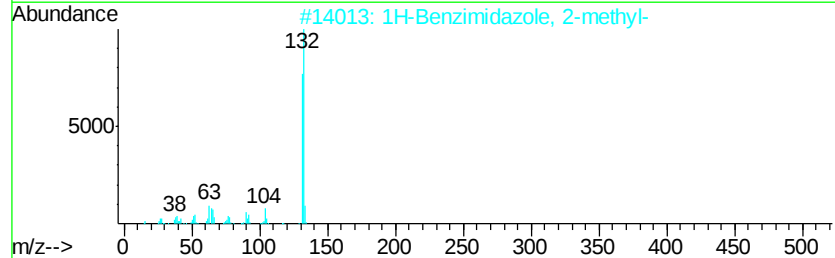
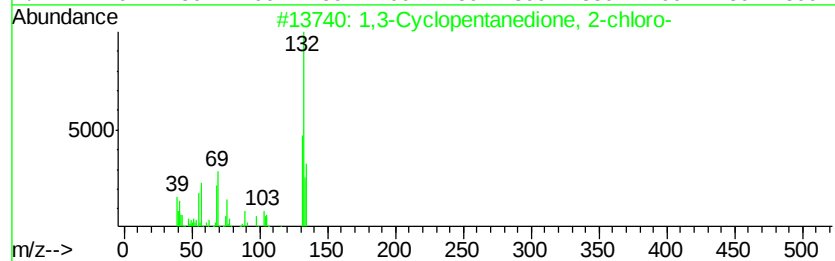
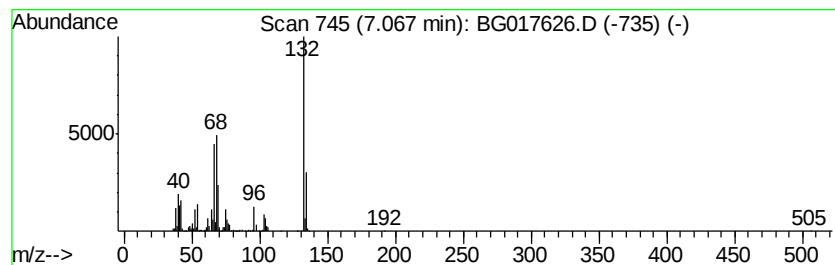
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown7.07 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.07	90.78 ng	715590	1,4-Dichlorobenzene-d4	7.53

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	16
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14
3		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
5		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14



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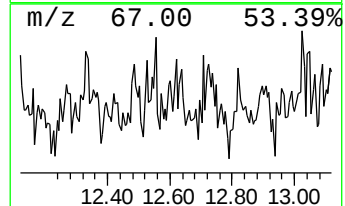
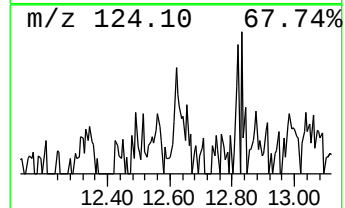
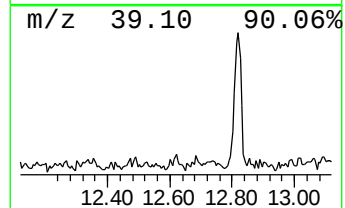
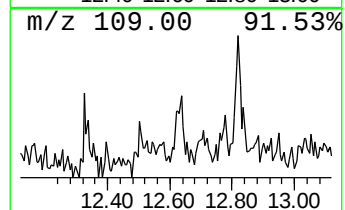
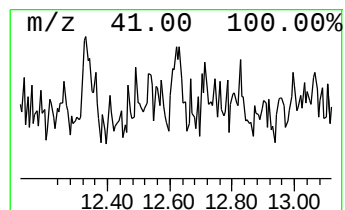
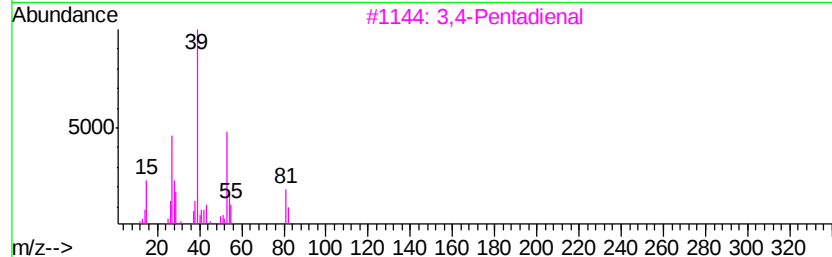
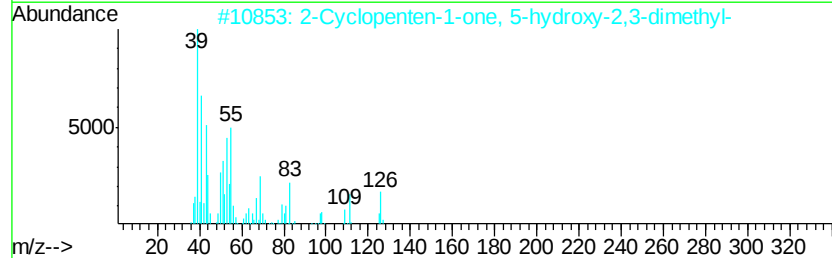
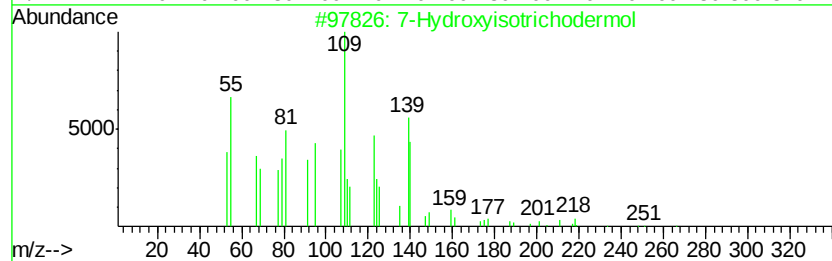
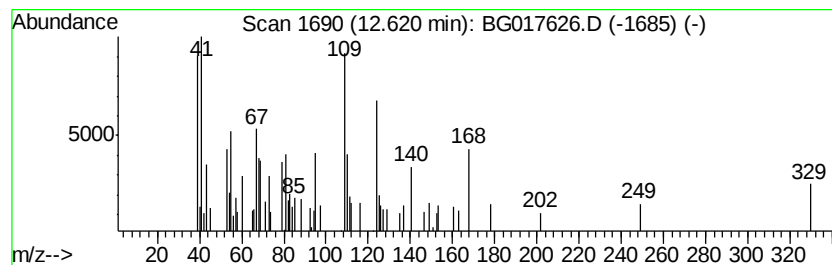
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 7-Hydroxyisotrichodermol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.62	2.06 ng	36733	Acenaphthene-d10	14.21	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Hydroxyisotrichodermol	266	C15H22O4	099624-08-5	53
2	2-Cyclopenten-1-one, 5-hydroxy-2...	126	C7H10O2	058649-31-3	49
3	3,4-Pentadienal	82	C5H6O	004009-55-6	47
4	Propane, 1-(2,2-dichloro-1,3,3-t...	194	C9H16Cl2	024551-93-7	47
5	Cyclohexene, 3,5,5-trimethyl-	124	C9H16	000933-12-0	47



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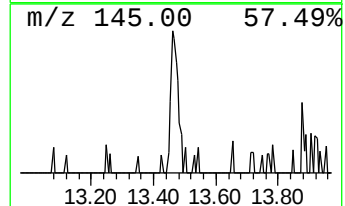
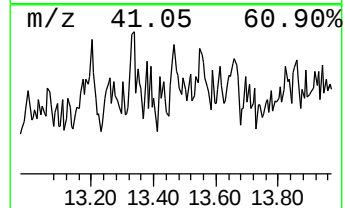
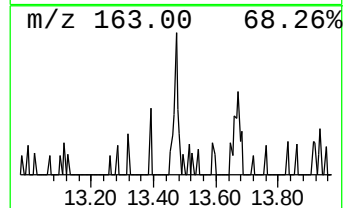
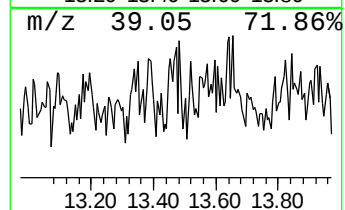
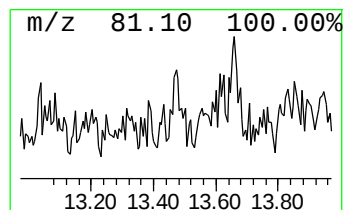
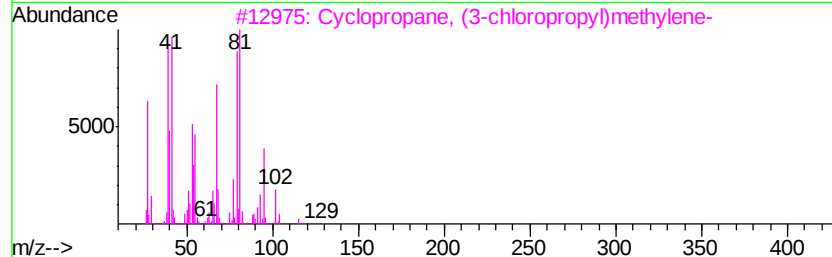
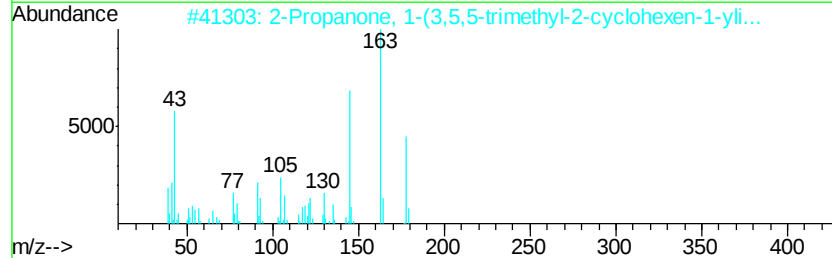
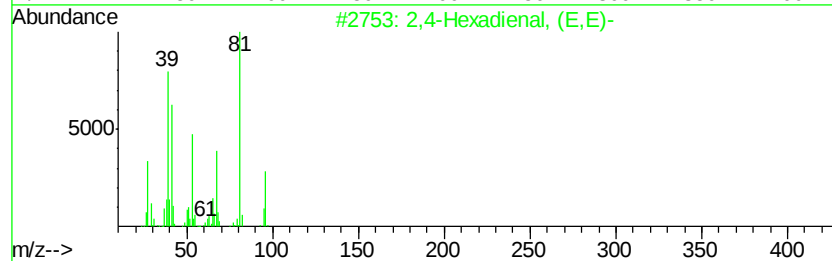
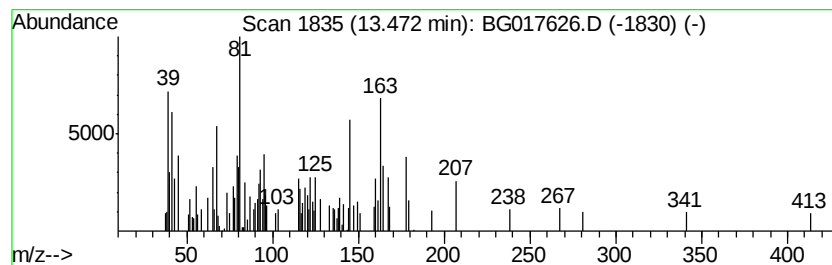
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Peak Number 5 unknown13.47 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.47	2.31 ng	41231	Acenaphthene-d10	14.21

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Hexadienal, (E,E)-			96	C6H8O	000142-83-6	25
2	2-Propanone, 1-(3,5,5-trimethyl-...			178	C12H18O	016695-73-1	22
3	Cyclopropane, (3-chloropropyl)me...			130	C7H11Cl	126755-04-2	12
4	Benzaldehyde, 2-hydroxy-5-nitro-			167	C7H5NO4	000097-51-8	11
5	1,3,3-Trimethyl-2-(2-methyl-cycl...			178	C13H22	285129-06-8	11



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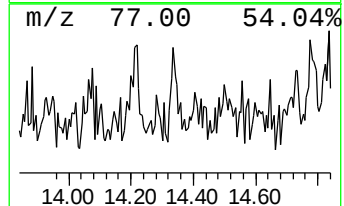
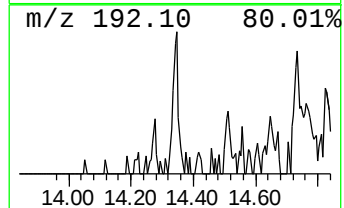
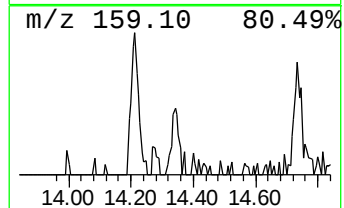
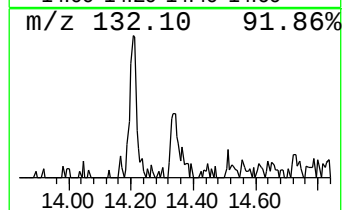
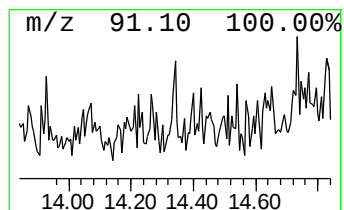
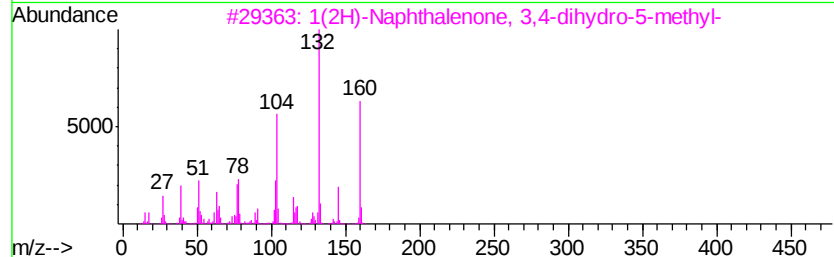
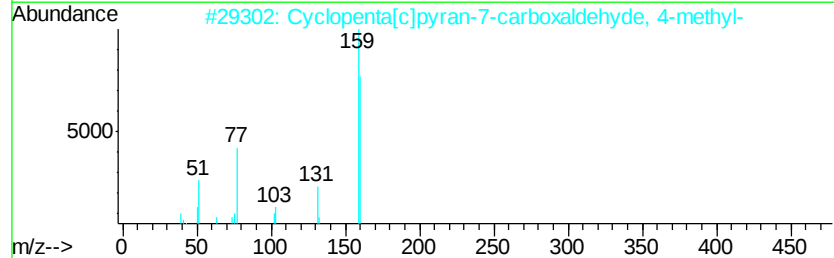
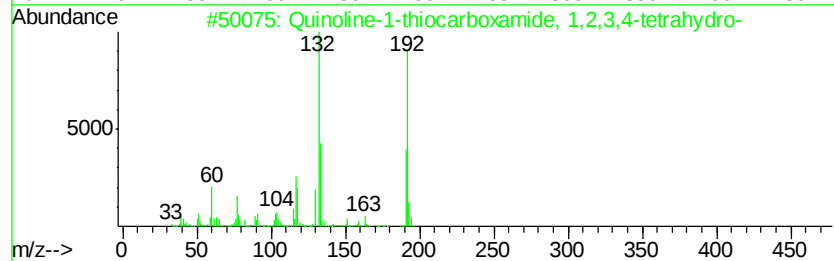
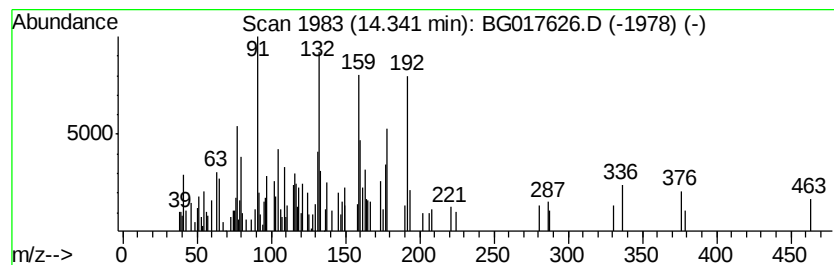
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown14.34 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.34	2.02 ng	36047	Acenaphthene-d10		14.21
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Quinoline-1-thiocarboxamide, 1,2...	192	C10H12N2S	262853-30-5	25
2	Cyclopenta[c]pyran-7-carboxaldeh...	160	C10H8O2	063661-79-0	25
3	1(2H)-Naphthalenone, 3,4-dihydro...	160	C11H12O	006939-35-1	18
4	cis-2-Methyl-4-phenylthiane	192	C12H16S	076097-69-3	18
5	2-Methyl-3-nitrobenzyl alcohol	167	C8H9NO3	023876-13-3	15



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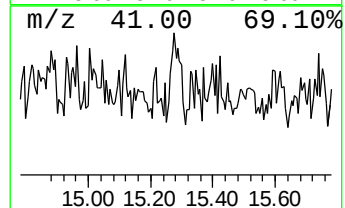
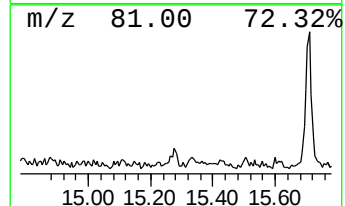
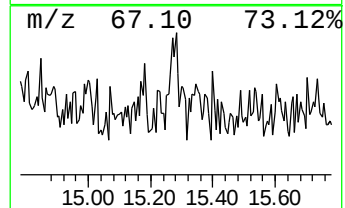
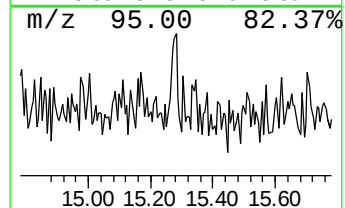
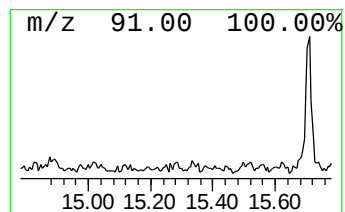
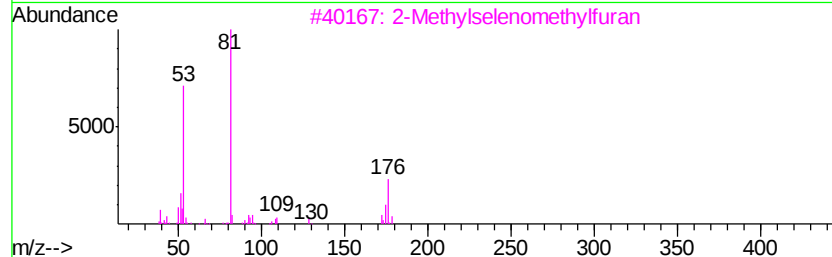
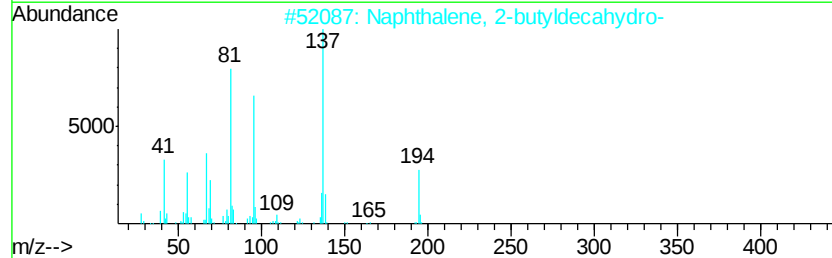
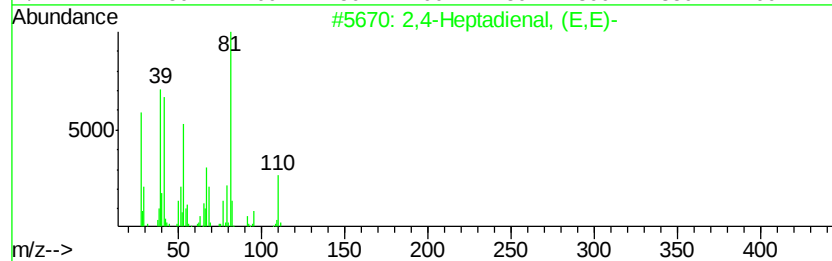
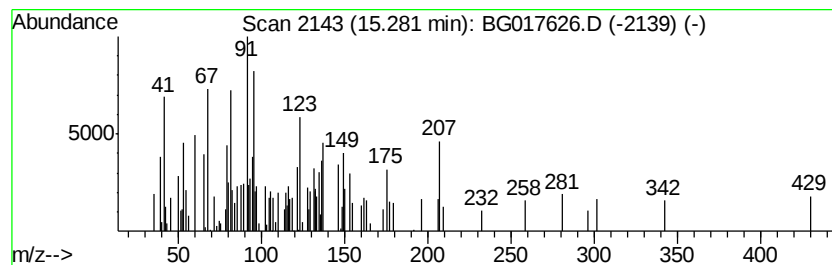
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown15.28 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.28	2.03 ng	36224	Acenaphthene-d10	14.21

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,4-Heptadienal, (E,E)-	110	C7H10O	004313-03-5	38
2		Naphthalene, 2-butyldecahydro-	194	C14H26	006305-52-8	25
3		2-Methylselenomethylfuran	176	C6H8OSe	209530-83-6	25
4		Bicyclo[3.2.2]non-6-en-3-one	136	C9H12O	1000072-31-7	25
5		3-Methylselenomethylfuran	176	C6H8OSe	209530-84-7	22



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG061115\
Data File : BG017626.D
Acq On : 12 Jun 2015 1:08
Operator : TP/IZ
Sample : G2523-12
Misc :
ALS Vial : 26 Sample Multiplier: 1

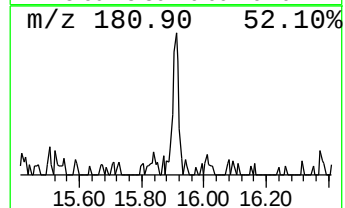
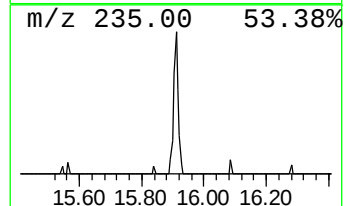
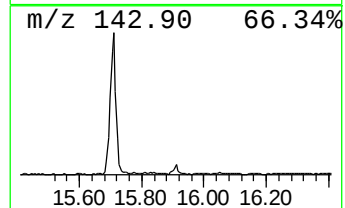
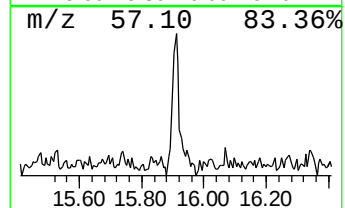
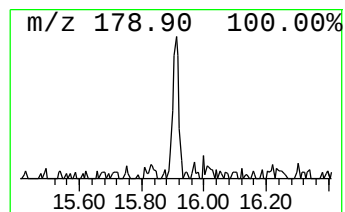
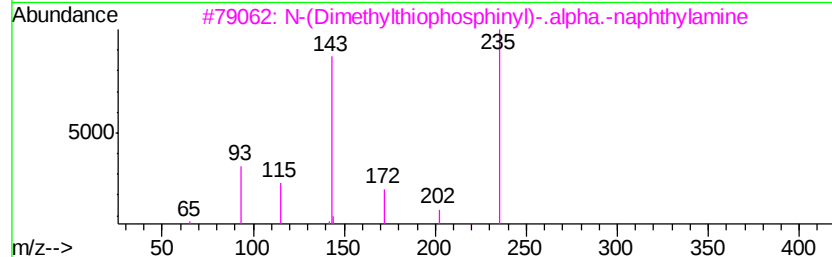
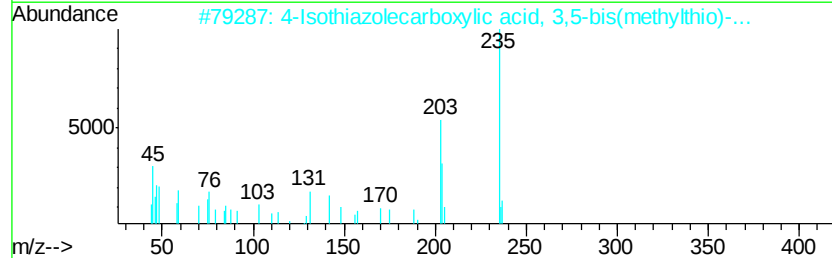
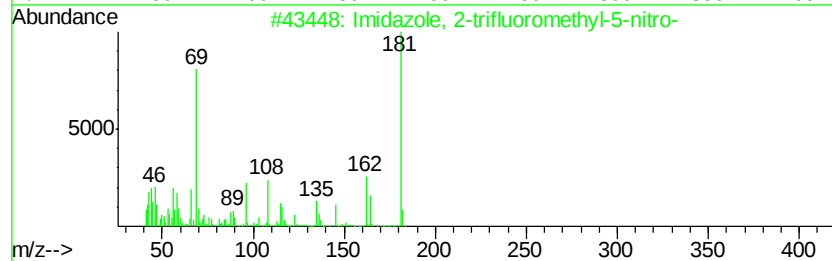
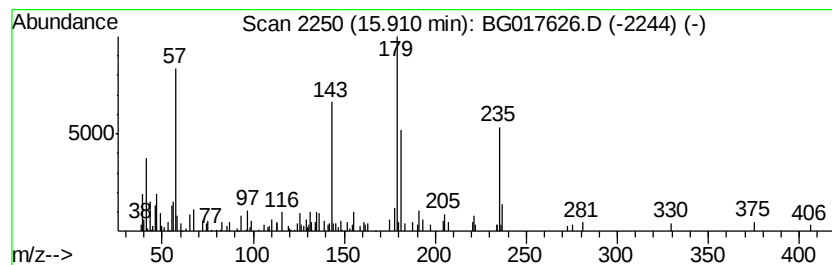
Instrument :
BNA_G
ClientSampleId :
PZ-6-6-4-15

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown15.91 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.91	2.82 ng	66769	Phenanthrene-d10	16.96	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Imidazole, 2-trifluoromethyl-5-n...	181	C4H2F3N3O2	104752-67-2	10
2	4-Isothiazolecarboxylic acid, 3,...	235	C7H9N02S3	002272-94-8	10
3	N-(Dimethylthiophosphinyl)-.alph...	235	C12H14NPS	069722-92-5	9
4	4-Chloro-2(1H)-quinolinone	179	C9H6ClNO	020146-59-2	9
5	2,4-Dimethoxyphenyl isocyanate	179	C9H9NO3	084370-87-6	9



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG061115\
Data File : BG017626.D
Acq On : 12 Jun 2015 1:08
Operator : TP/IZ
Sample : G2523-12
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PZ-6-6-4-15

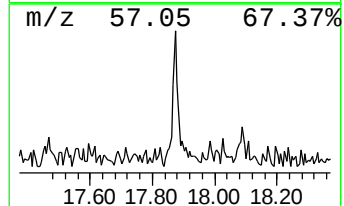
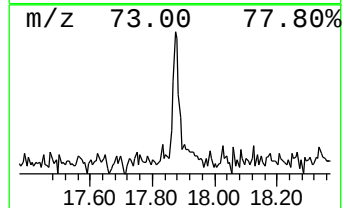
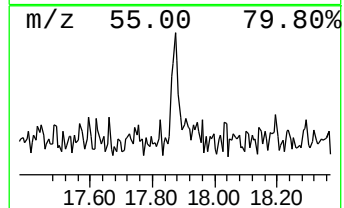
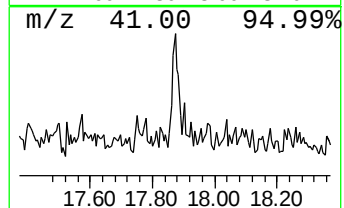
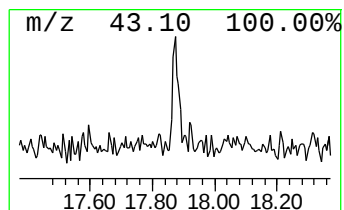
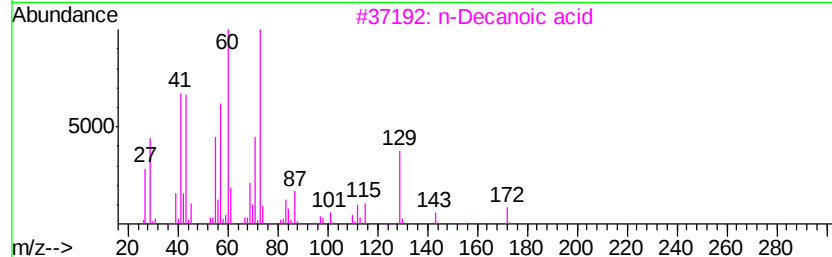
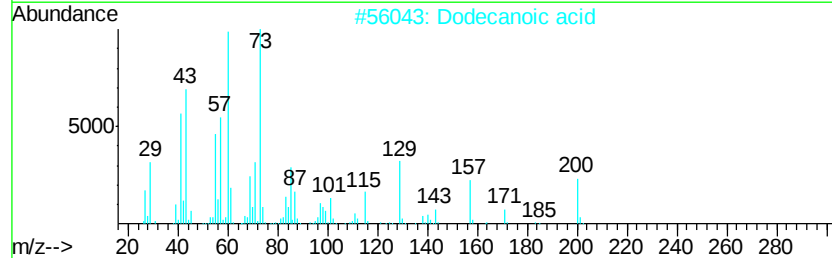
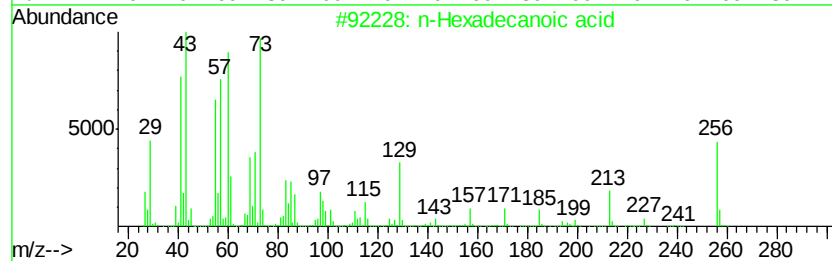
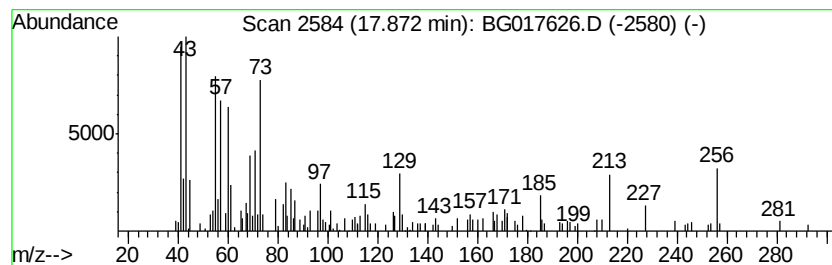
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.87	3.28 ng	77734	Phenanthrene-d10	16.96

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
2		Dodecanoic acid	200	C12H24O2	000143-07-7	49
3		n-Decanoic acid	172	C10H20O2	000334-48-5	47
4		D-Glucose, 4-O-.alpha.-D-glucopy...	342	C12H22O11	000069-79-4	43
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	43



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG061115\
Data File : BG017626.D
Acq On : 12 Jun 2015 1:08
Operator : TP/IZ
Sample : G2523-12
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PZ-6-6-4-15

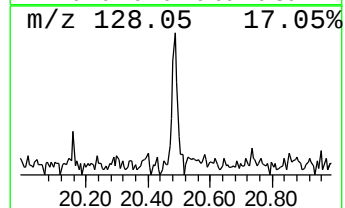
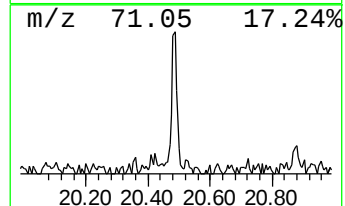
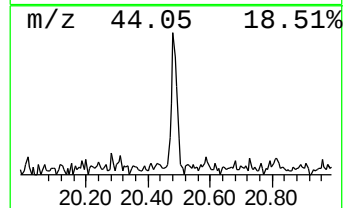
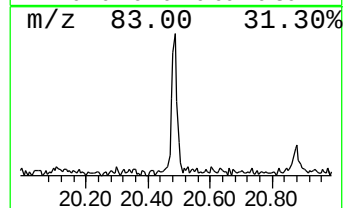
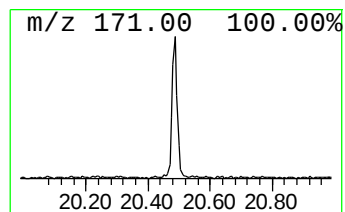
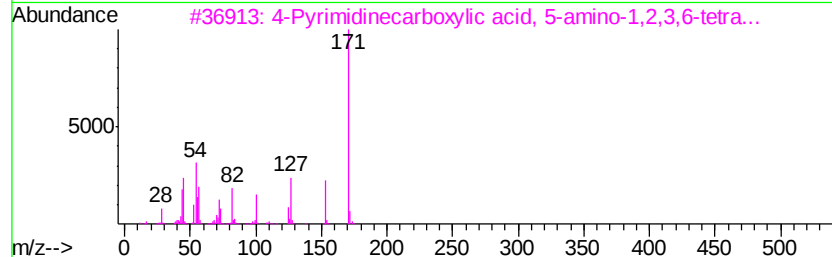
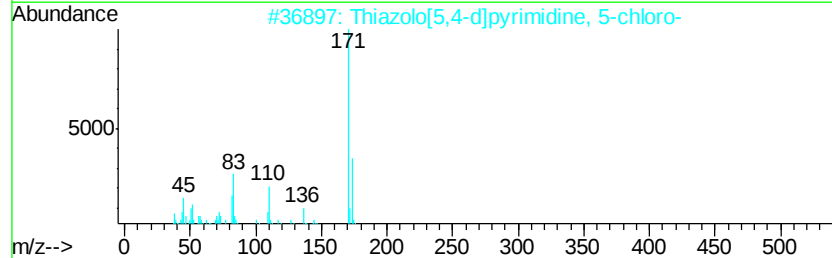
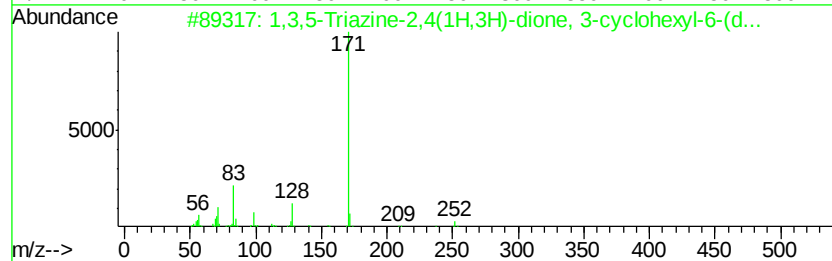
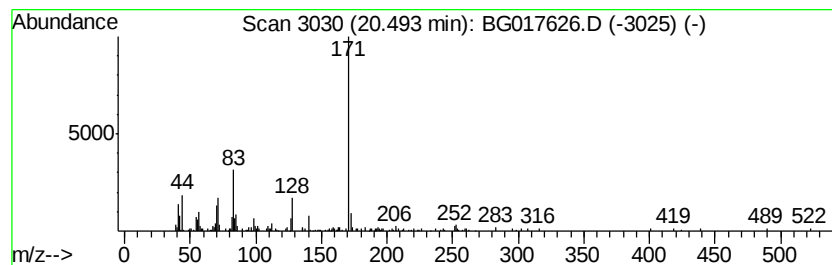
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1,3,5-Triazine-2,4(1H,3H)-d... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.49	4.63 ng	133094	Chrysene-d12	21.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3,5-Triazine-2,4(1H,3H)-dione, ...	252	C12H20N4O2	051235-04-2	91
2		Thiazolo[5,4-d]pyrimidine, 5-chl...	171	C5H2ClN3S	013316-08-0	64
3		4-Pyrimidinecarboxylic acid, 5-a...	171	C5H5N3O4	007164-43-4	50
4		2,4(1H,3H)-Pyrimidinedione, 6-me...	171	C5H5N3O4	016632-21-6	50
5		Benzeneethanamine, 2-fluoro-4-hy...	171	C8H10FN02	1000116-43-3	45



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG061115\
Data File : BG017626.D
Acq On : 12 Jun 2015 1:08
Operator : TP/IZ
Sample : G2523-12
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PZ-6-6-4-15

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060315.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...	4.63	4.1 ng		32559	1	7.53	157655	20.0
unknown7.07	7.07	90.8 ng		715590	1	7.53	157655	20.0
7-Hydroxyisotrich...	12.62	2.1 ng		36733	3	14.21	356900	20.0
unknown13.47	13.47	2.3 ng		41231	3	14.21	356900	20.0
unknown14.34	14.34	2.0 ng		36047	3	14.21	356900	20.0
unknown15.28	15.28	2.0 ng		36224	3	14.21	356900	20.0
unknown15.91	15.91	2.8 ng		66769	4	16.96	473848	20.0
n-Hexadecanoic acid	17.87	3.3 ng		77734	4	16.96	473848	20.0
1,3,5-Triazine-2,...	20.49	4.6 ng		133094	5	21.16	574766	20.0