

Data Path : Z:\HPCHEM1\BNA G\DATA\BG072716\
 Data File : BG023287.D
 Acq On : 27 Jul 2016 17:42
 Operator : UM/SJ
 Sample : H4152-10
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 GW-16-7.0-15.0

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_G\METHODS\8270-BG072616.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	4.180	216	228	235	rBV2	238798	652681	5.22%	0.884%
2	4.285	240	246	254	rVB2	92564	174246	1.39%	0.236%
3	5.196	394	401	410	rVB2	202711	318864	2.55%	0.432%
4	5.672	473	482	495	rBV	2098001	3415632	27.31%	4.624%
5	7.287	750	757	768	rVB	1554430	2721432	21.76%	3.684%
6	7.663	813	821	830	rBV	3109338	5423185	43.35%	7.342%
7	8.133	895	901	908	rBV	761505	1315453	10.52%	1.781%
8	8.374	934	942	949	rBV	68073	138919	1.11%	0.188%
9	8.462	949	957	966	rVB	2619506	4517115	36.11%	6.115%
10	9.314	1094	1102	1114	rVB	2388077	4208976	33.65%	5.698%
11	10.970	1377	1384	1391	rBV	1051372	1940166	15.51%	2.627%
12	13.420	1793	1801	1811	rBV	5920452	9663827	77.25%	13.083%
13	14.248	1937	1942	1948	rBV	244102	356735	2.85%	0.483%
14	14.806	2029	2037	2044	rBV2	1652362	2758991	22.06%	3.735%
15	14.871	2044	2048	2057	rVB2	94987	156931	1.25%	0.212%
16	15.323	2120	2125	2132	rBV2	88334	153635	1.23%	0.208%
17	15.494	2149	2154	2158	rVB	178382	256088	2.05%	0.347%
18	16.257	2276	2284	2286	rBV	198973	282464	2.26%	0.382%
19	16.304	2286	2292	2305	rVB	5068454	7700496	61.56%	10.425%
20	16.962	2399	2404	2410	rBV	72962	136117	1.09%	0.184%
21	17.274	2452	2457	2467	rBV6	153724	391368	3.13%	0.530%
22	17.567	2494	2507	2512	rBV2	2116017	3633395	29.05%	4.919%
23	17.614	2512	2515	2519	rVB	188037	253930	2.03%	0.344%
24	18.443	2652	2656	2663	rBV3	122529	239714	1.92%	0.325%
25	18.678	2689	2696	2704	rBV	2139434	3075967	24.59%	4.164%
26	18.778	2710	2713	2722	rVB9	101494	167872	1.34%	0.227%
27	19.717	2869	2873	2884	rBV9	74089	212426	1.70%	0.288%
28	20.182	2945	2952	2957	rBV	9315859	12509079	100.00%	16.935%
29	21.891	3236	3243	3252	rVB	2127749	3706543	29.63%	5.018%
30	25.298	3812	3823	3836	rBV	1143595	3381938	27.04%	4.579%

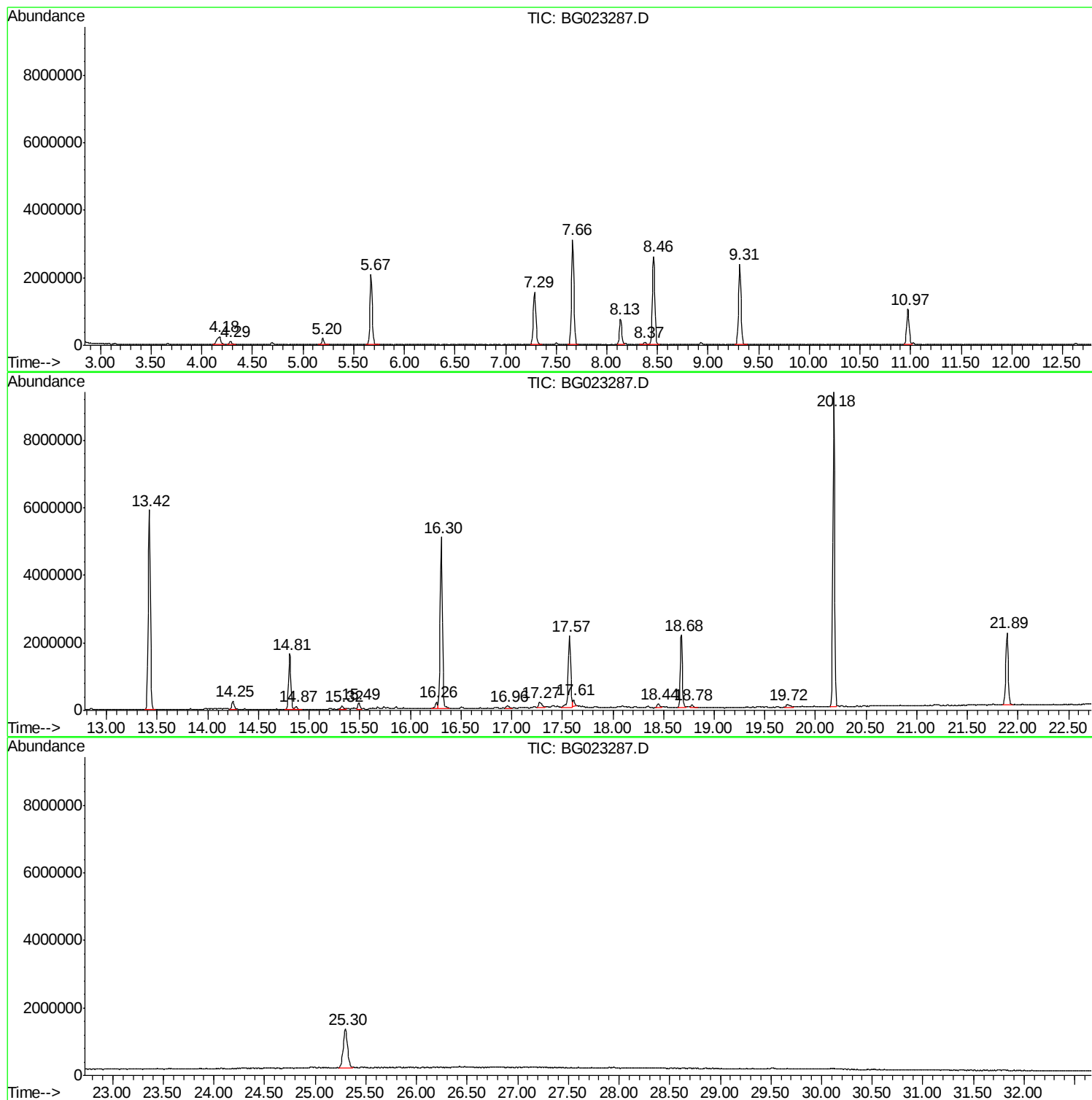
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Instrument :
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ClientSampleId :
GW-16-7.0-15.0

Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG072616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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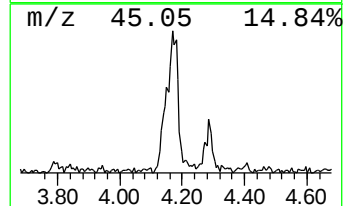
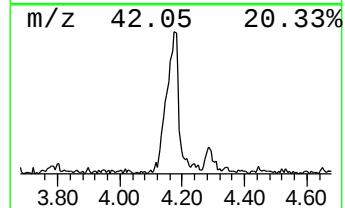
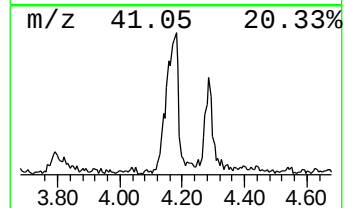
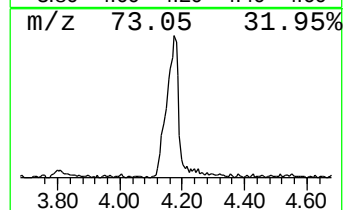
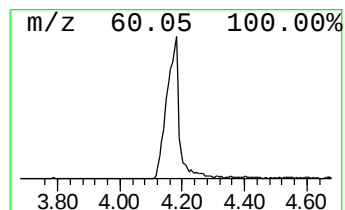
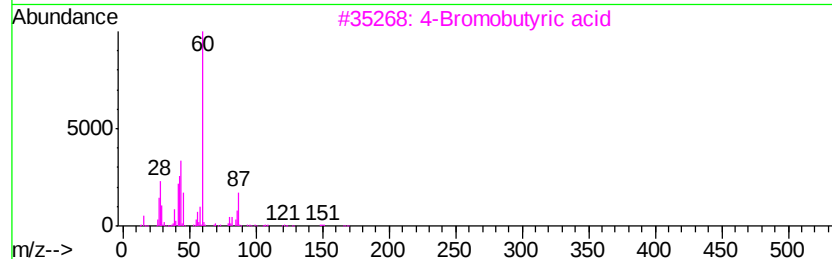
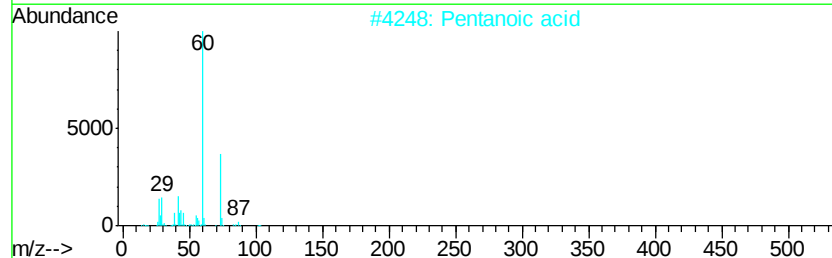
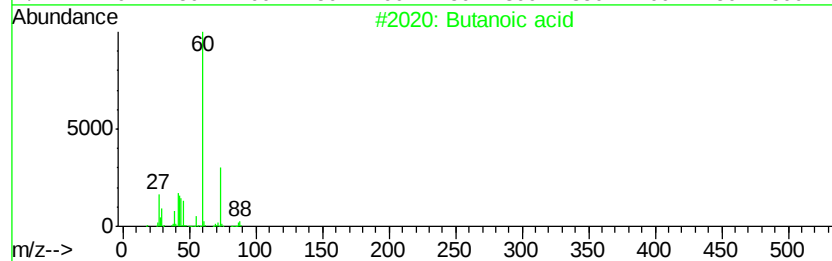
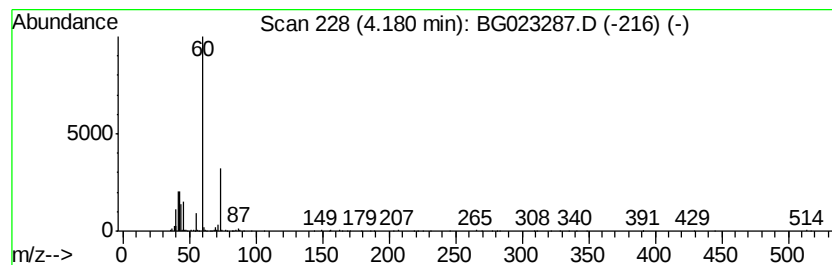
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.18	9.92 ng	652681	1,4-Dichlorobenzene-d4	8.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanoic acid	88	C4H8O2	000107-92-6	64
2		Pentanoic acid	102	C5H10O2	000109-52-4	45
3		4-Bromobutvric acid	166	C4H7BrO2	002623-87-2	9
4		Urea	60	CH4N2O	000057-13-6	5
5		Formic acid hydrazide	60	CH4N2O	000624-84-0	4



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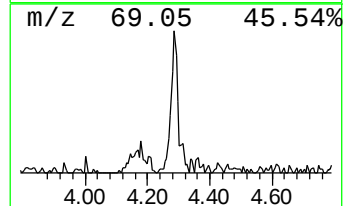
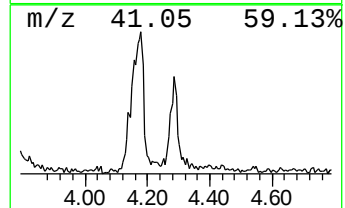
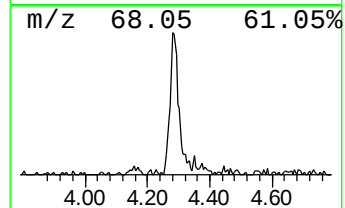
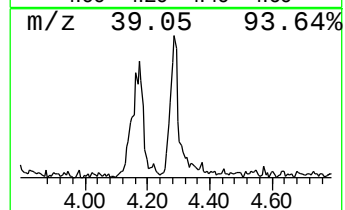
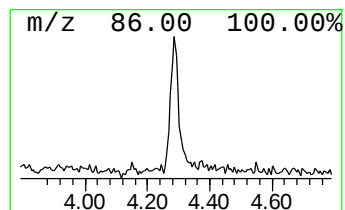
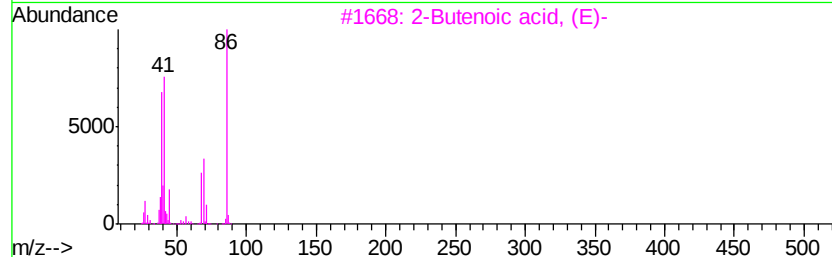
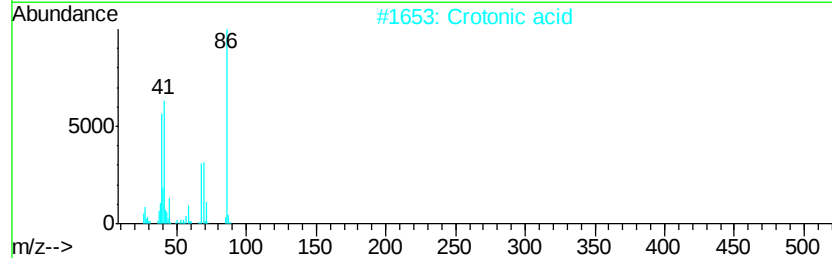
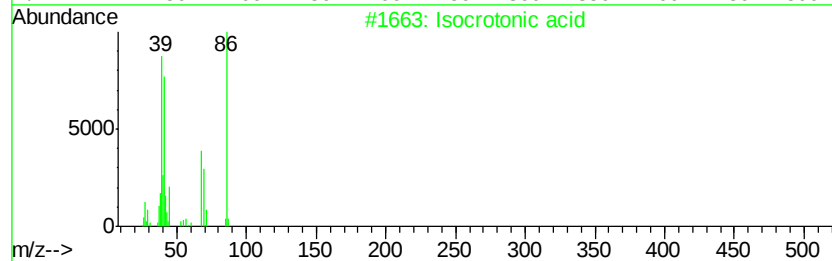
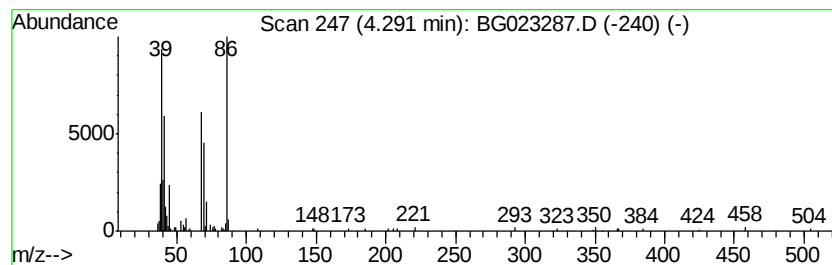
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Peak Number 2 Isocrotonic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.29	2.65 ng	174246	1,4-Dichlorobenzene-d4	8.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isocrotonic acid	86	C4H6O2	000503-64-0	94
2		Crotonic acid	86	C4H6O2	003724-65-0	91
3		2-Butenoic acid, (E)-	86	C4H6O2	000107-93-7	90
4		2-Propenoic acid, 2-methyl-	86	C4H6O2	000079-41-4	87
5		cis-4-Hydroxy-L-proline	131	C5H9NO3	000618-27-9	64



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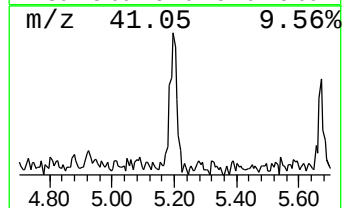
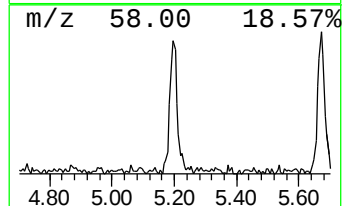
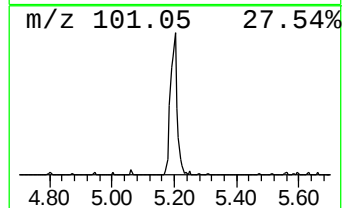
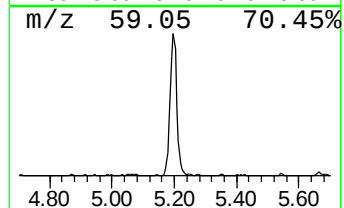
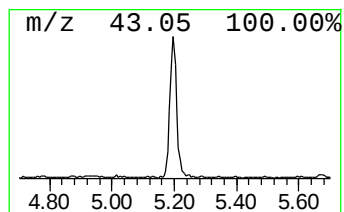
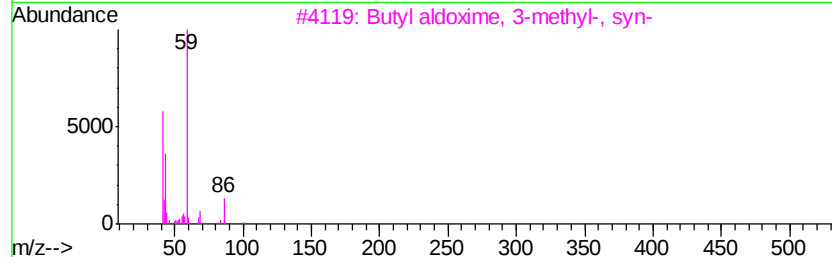
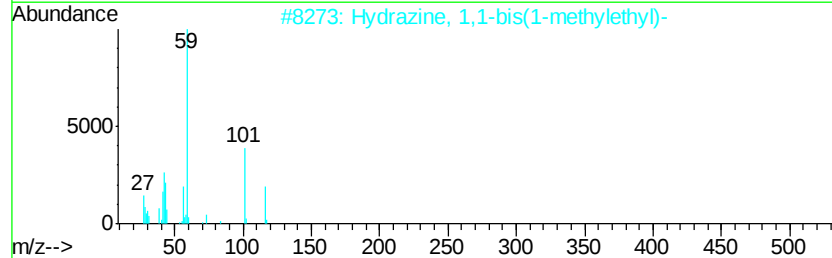
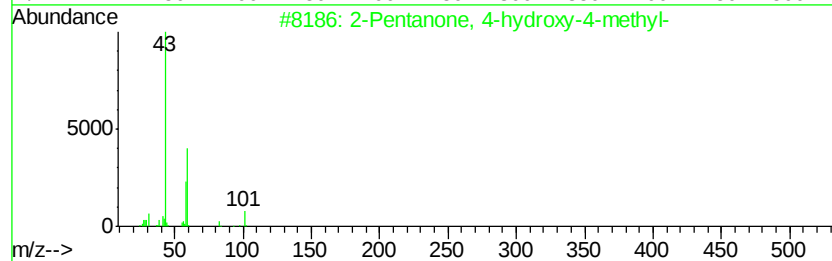
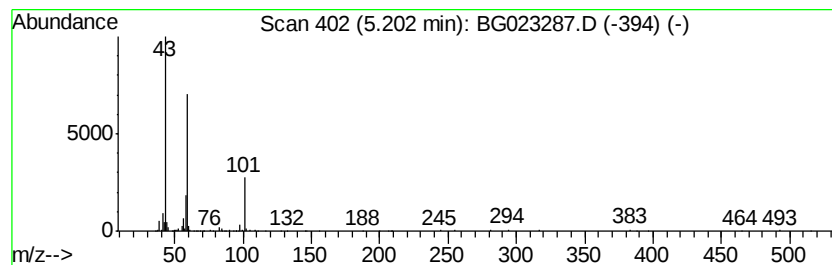
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	4.85 ng	318864	1,4-Dichlorobenzene-d4	8.13

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2		000123-42-2	59
2	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2		000921-14-2	25
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO		005780-40-5	12
4	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2		001116-98-9	12
5	Guanidine	59	CH5N3		000113-00-8	9



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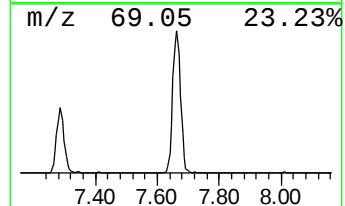
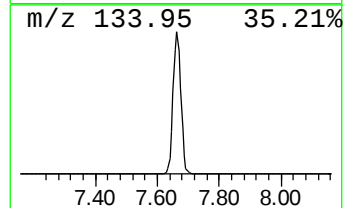
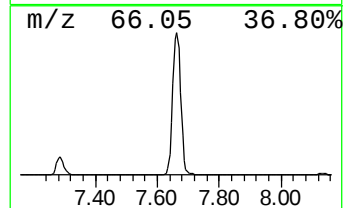
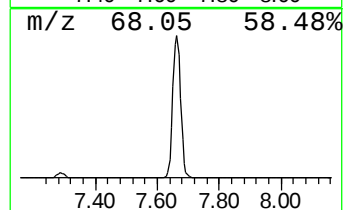
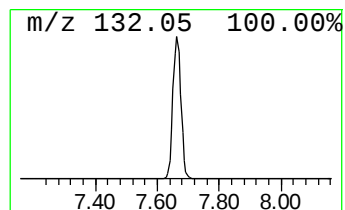
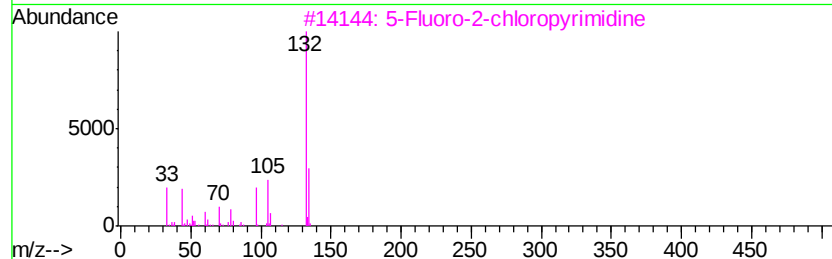
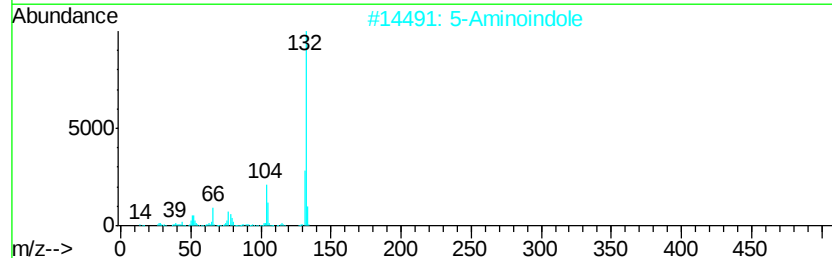
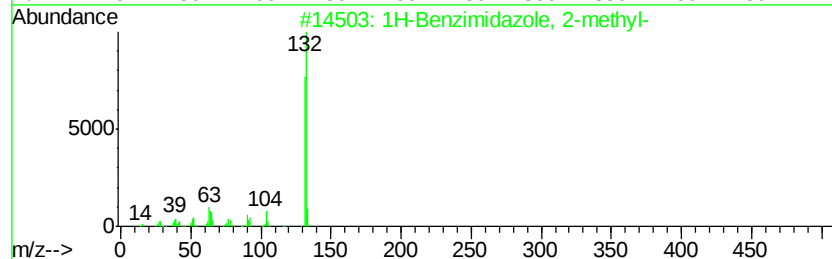
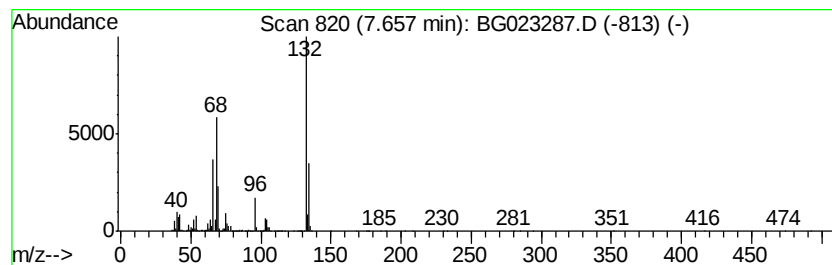
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Peak Number 4 unknown7.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.66	82.45 ng	5423190	1,4-Dichlorobenzene-d4	8.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
2		5-Aminoindole	132	C8H8N2	005192-03-0	22
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	11
5		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10



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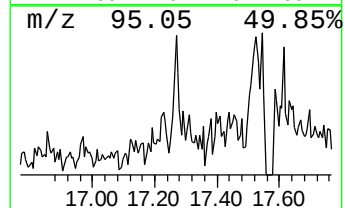
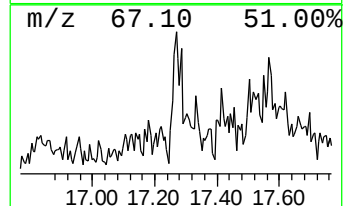
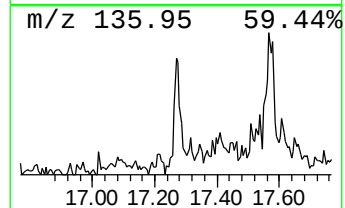
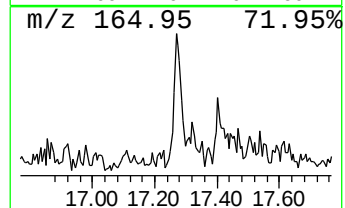
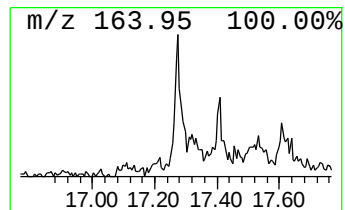
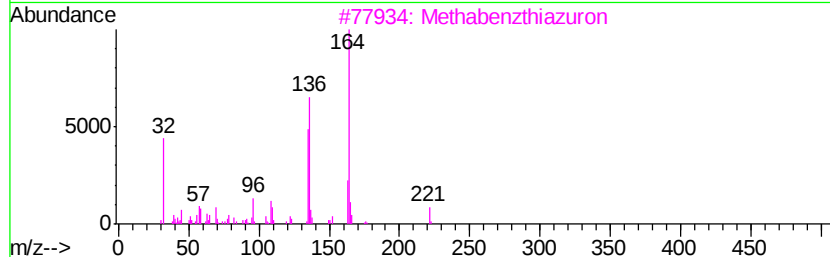
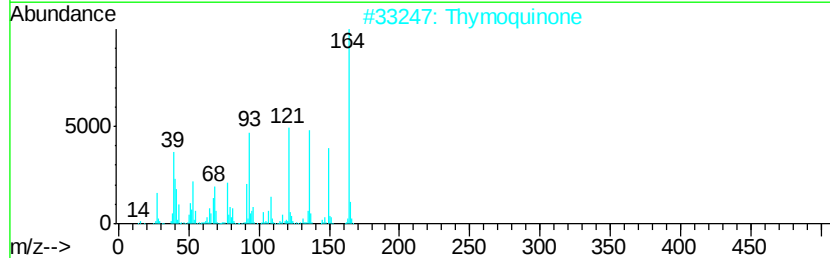
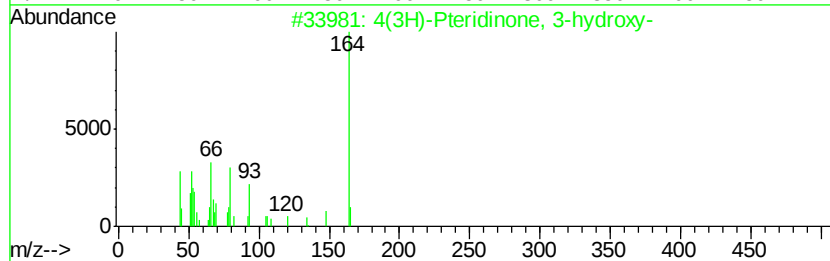
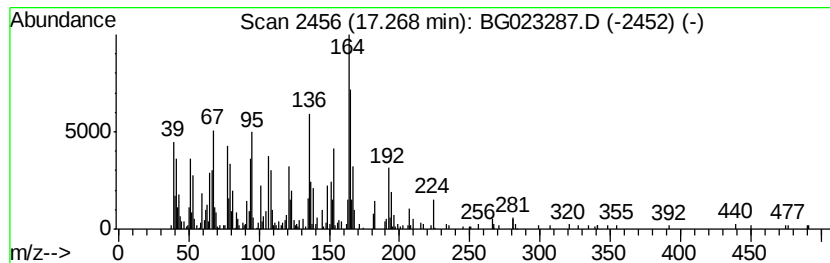
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Peak Number 6 unknown17.27 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.27	2.15 ng	391368	Phenanthrene-d10	17.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4(3H)-Pteridinone, 3-hydroxy-	164	C6H4N4O2	018106-57-5	38
2		Thymoquinone	164	C10H12O2	000490-91-5	22
3		Methabenzthiazuron	221	C10H11N3OS	018691-97-9	22
4		Benzoic acid, 4-(dimethylamino)-	165	C9H11NO2	000619-84-1	14
5		Propionic acid, 3-(4-cyclopentyl...	368	C21H24N2O4	1000311-07-5	14



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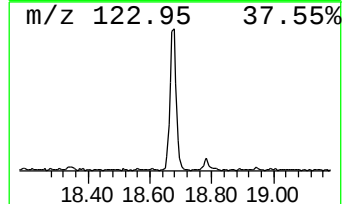
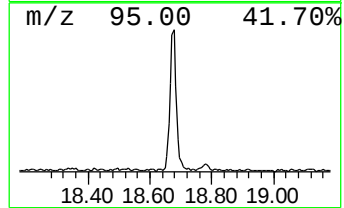
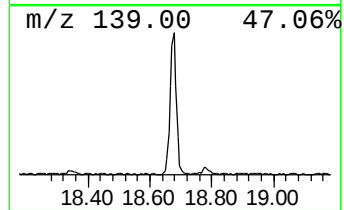
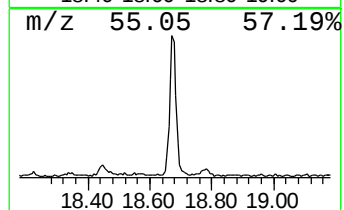
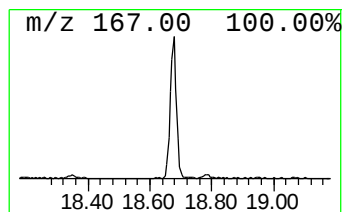
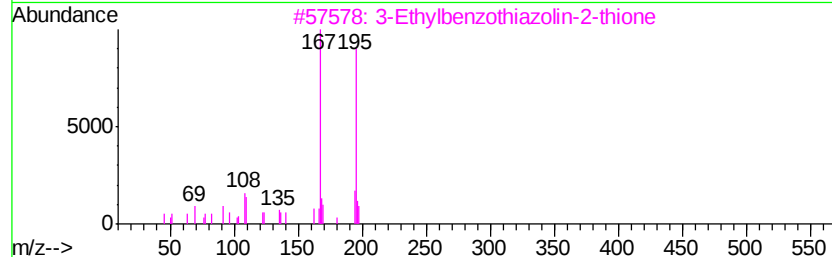
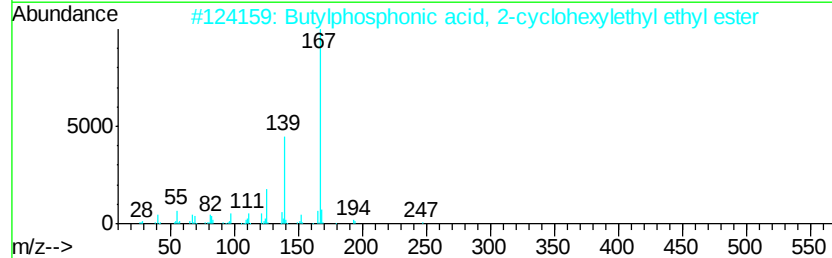
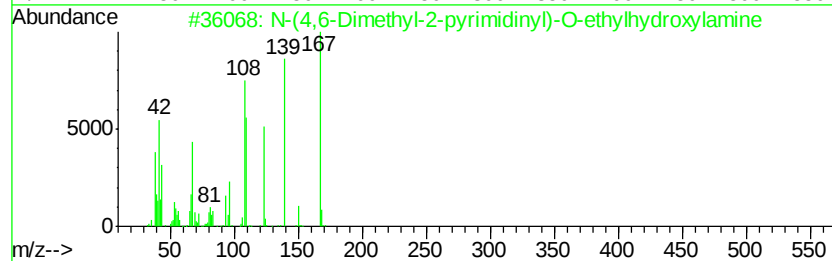
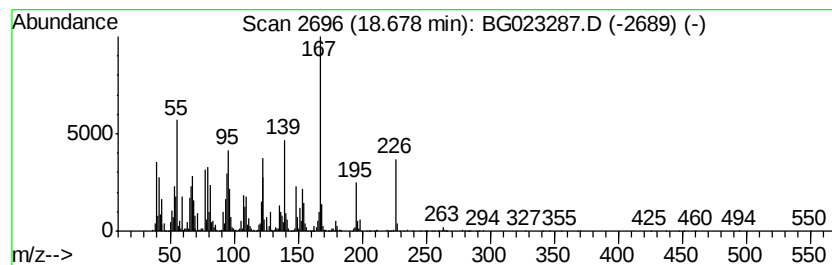
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG072616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown18.68 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.68	16.93 ng	3075970	Phenanthrene-d10	17.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	N-(4,6-Dimethyl-2-pyrimidinyl)-O...	167	C8H13N3O	300358-25-2	27
2		Butylphosphonic acid, 2-cyclohex...	276	C14H29O3P	1000323-20-5	22
3		3-Ethylbenzothiazolin-2-thione	195	C9H9NS2	016407-34-4	18
4		4,8-Ethano-4H-1,3-benzodioxin, h...	168	C10H16O2	057790-44-0	15
5		2-Mercaptobenzothiazole	167	C7H5NS2	000149-30-4	14



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG072716\
Data File : BG023287.D
Acq On : 27 Jul 2016 17:42
Operator : UM/SJ
Sample : H4152-10
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GW-16-7.0-15.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG072616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butanoic acid	4.18	9.9	ng	652681	1	8.13	1315450	20.0
Isocrotonic acid	4.29	2.6	ng	174246	1	8.13	1315450	20.0
2-Pentanone, 4-hy...	5.20	4.8	ng	318864	1	8.13	1315450	20.0
unknown7.66	7.66	82.5	ng	5423190	1	8.13	1315450	20.0
unknown17.27	17.27	2.1	ng	391368	4	17.57	3633400	20.0
unknown18.68	18.68	16.9	ng	3075970	4	17.57	3633400	20.0