

Data Path : Z:\HPCHEM1\BNA G\DATA\BG110416\
 Data File : BG024706.D
 Acq On : 5 Nov 2016 10:47
 Operator : UM/SJ
 Sample : H5509-24
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 GW-94-8.8-20.0

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-BG102516.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	3.196	56	61	67	rBV	82804	123701	1.25%	0.207%
2	3.601	123	130	148	rVB	2097309	4041990	40.70%	6.761%
3	5.329	418	424	432	rVB	206194	336370	3.39%	0.563%
4	5.799	497	504	514	rVB	1139088	1949018	19.63%	3.260%
5	6.310	581	591	599	rBV	4079096	6975212	70.24%	11.667%
6	7.226	738	747	758	rBV4	61307	152932	1.54%	0.256%
7	7.403	769	777	790	rVB	783594	1430820	14.41%	2.393%
8	7.791	834	843	857	rBV	1936922	3802009	38.28%	6.359%
9	8.266	917	924	933	rBV	443627	777307	7.83%	1.300%
10	8.590	971	979	987	rBV	1727678	3137231	31.59%	5.248%
11	9.442	1116	1124	1131	rBV	1510695	2810337	28.30%	4.701%
12	9.571	1141	1146	1154	rVB3	80625	133556	1.34%	0.223%
13	11.093	1395	1405	1419	rVB	553791	1211410	12.20%	2.026%
14	11.839	1525	1532	1542	rBV4	69337	154161	1.55%	0.258%
15	13.507	1809	1816	1824	rVB	3863213	6065684	61.08%	10.146%
16	14.882	2041	2050	2056	rBV	953663	1472198	14.82%	2.462%
17	16.363	2295	2302	2314	rBV	3710388	6028086	60.70%	10.083%
18	17.274	2451	2457	2462	rVB5	50259	100672	1.01%	0.168%
19	17.626	2509	2517	2521	rBV	1276591	2033953	20.48%	3.402%
20	17.667	2521	2524	2530	rVB	327746	450574	4.54%	0.754%
21	18.020	2577	2584	2590	rBV	80387	143266	1.44%	0.240%
22	19.659	2859	2863	2868	rVB	152815	205656	2.07%	0.344%
23	19.865	2894	2898	2905	rBV2	133841	168629	1.70%	0.282%
24	20.023	2921	2925	2928	rBV	73288	107784	1.09%	0.180%
25	20.205	2950	2956	2962	rBV	7487359	9930825	100.00%	16.611%
26	20.781	3050	3054	3061	rBV	62737	117298	1.18%	0.196%
27	20.905	3072	3075	3079	rVB2	111552	123898	1.25%	0.207%
28	21.498	3172	3176	3184	rVB10	75669	125178	1.26%	0.209%
29	21.921	3240	3248	3255	rBV	1566970	2886415	29.07%	4.828%
30	25.352	3820	3832	3842	rVB2	904505	2788942	28.08%	4.665%

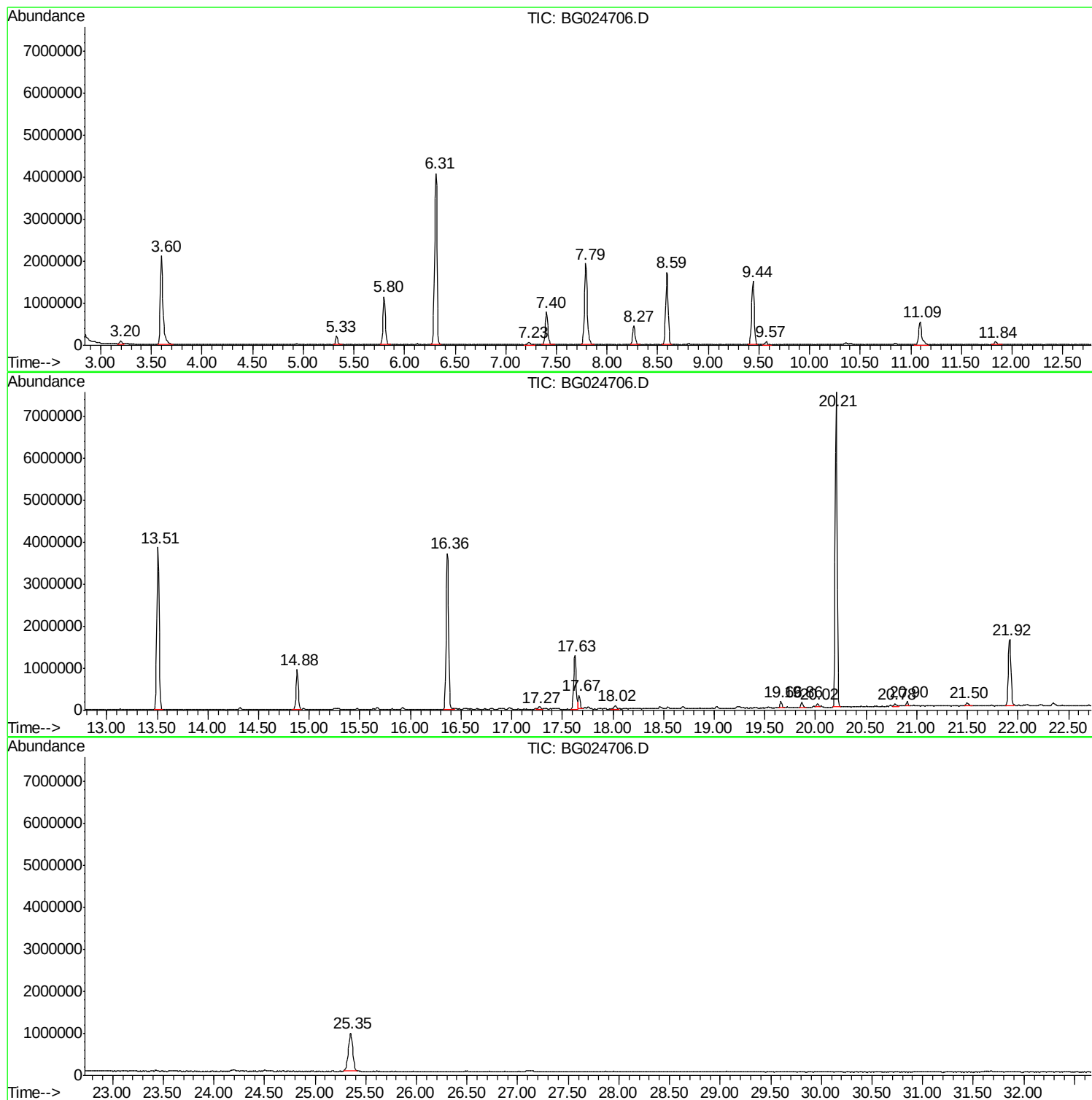
Sum of corrected areas: 59785112

Data Path : Z:\HPCHEM1\BNA G\DATA\BG110416\
Data File : BG024706.D
Acq On : 5 Nov 2016 10:47
Operator : UM/SJ
Sample : H5509-24
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GW-94-8.8-20.0

Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA G\DATA\BG110416\
Data File : BG024706.D
Acq On : 5 Nov 2016 10:47
Operator : UM/SJ
Sample : H5509-24
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GW-94-8.8-20.0

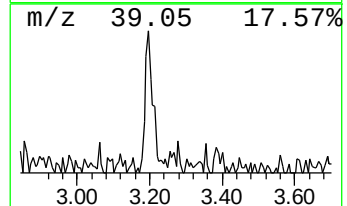
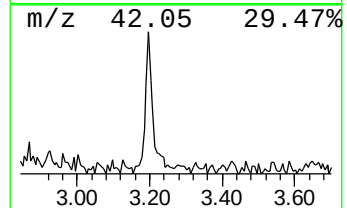
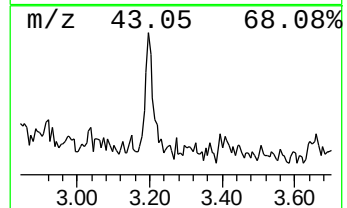
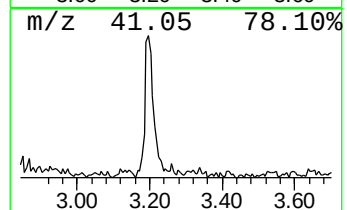
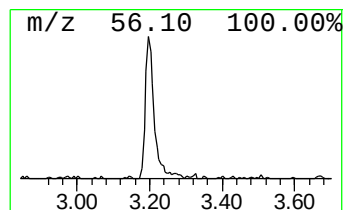
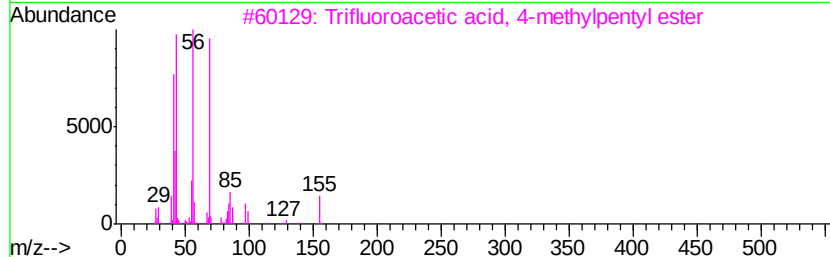
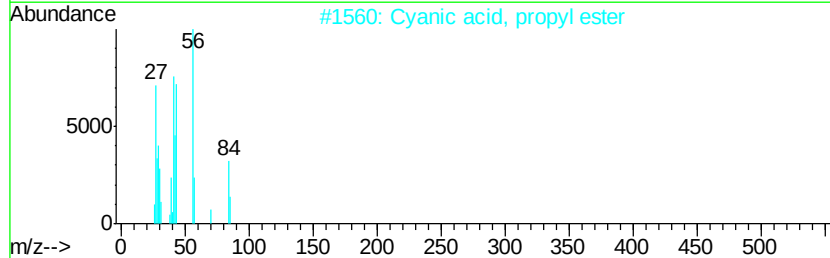
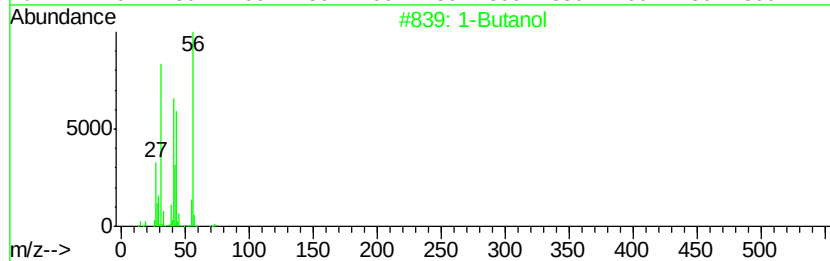
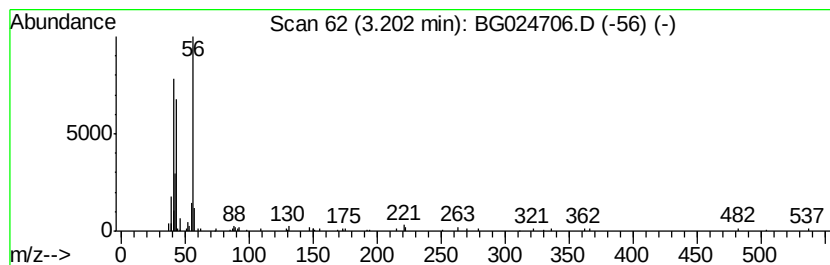
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1-Butanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.20	3.18 ng	123701	1,4-Dichlorobenzene-d4	8.26

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanol	74	C4H10O	000071-36-3	80
2			Cyanic acid, propyl ester	85	C4H7NO	001768-36-1	56
3			Trifluoroacetic acid, 4-methylpe...	198	C8H13F3O2	000327-71-9	56
4			Hexyl chloroformate	164	C7H13ClO2	006092-54-2	40
5			1-Hexanol	102	C6H14O	000111-27-3	40



Data Path : Z:\HPCHEM1\BNA G\DATA\BG110416\
Data File : BG024706.D
Acq On : 5 Nov 2016 10:47
Operator : UM/SJ
Sample : H5509-24
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GW-94-8.8-20.0

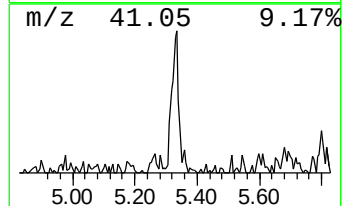
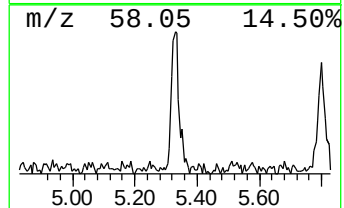
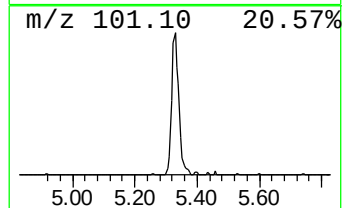
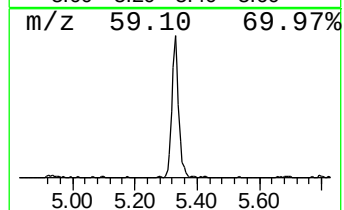
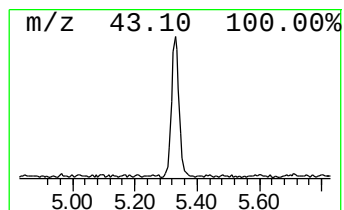
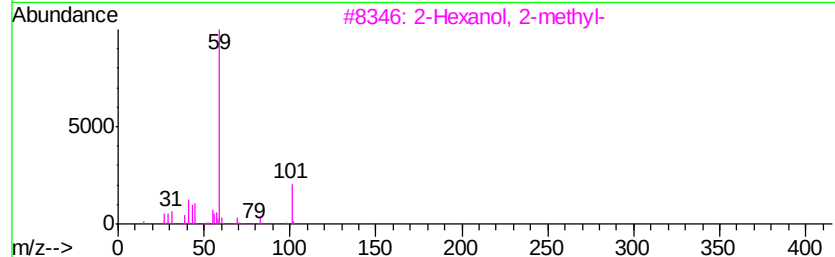
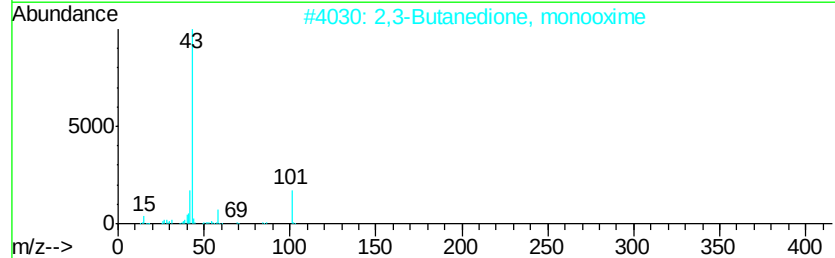
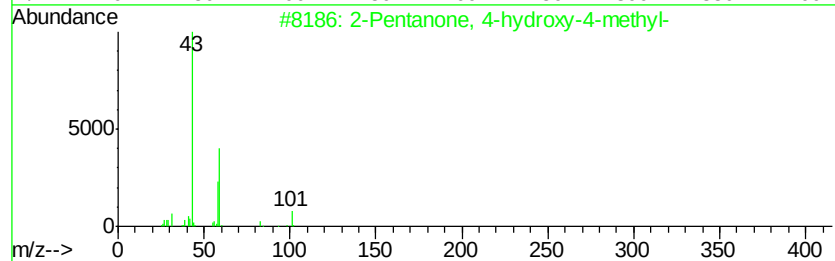
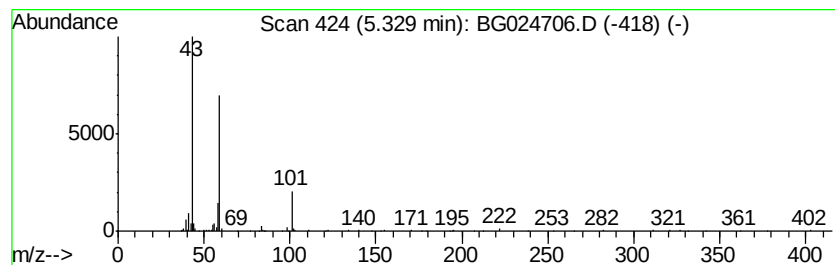
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.33	8.65 ng	336370	1,4-Dichlorobenzene-d4	8.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5		2,3-Dimethyloxirane-2-carboxylic...	130	C6H10O3	1000306-64-4	9



Data Path : Z:\HPCHEM1\BNA G\DATA\BG110416\
Data File : BG024706.D
Acq On : 5 Nov 2016 10:47
Operator : UM/SJ
Sample : H5509-24
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GW-94-8.8-20.0

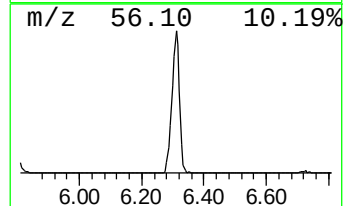
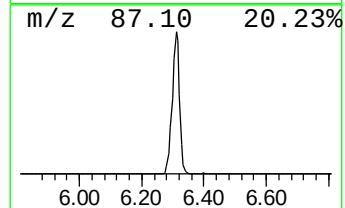
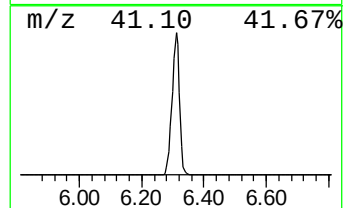
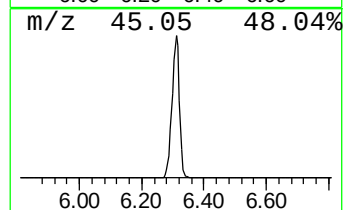
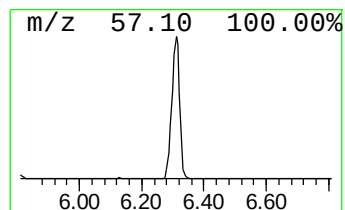
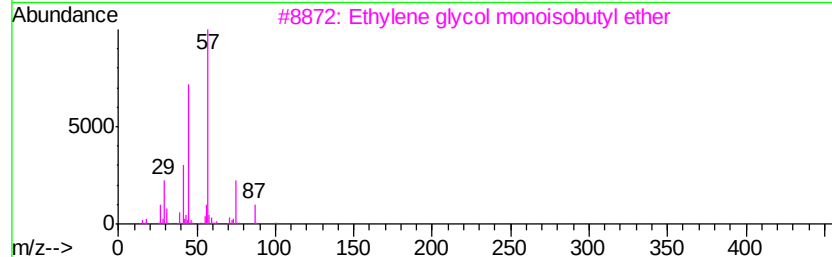
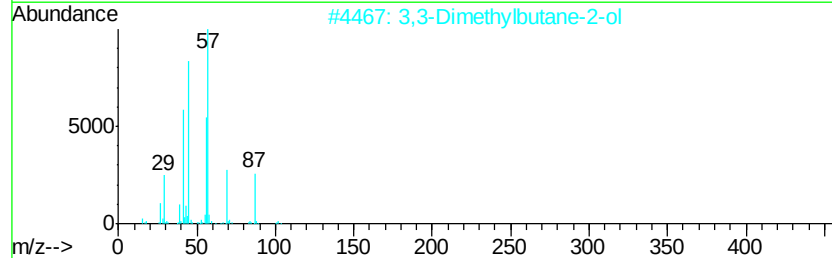
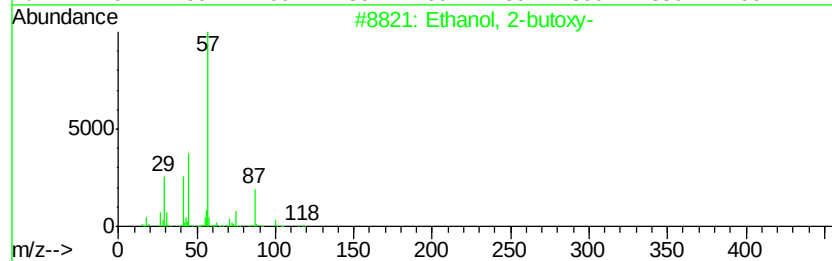
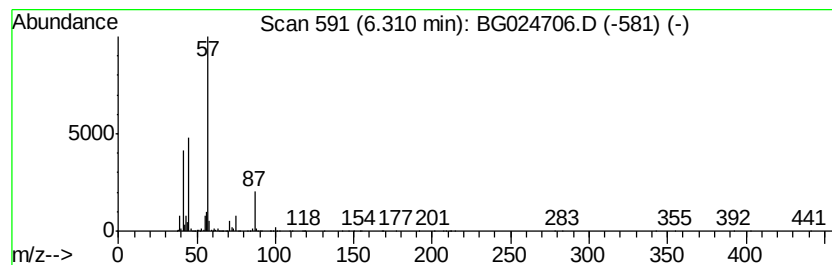
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Ethanol, 2-butoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.31	179.47 ng	6975210	1,4-Dichlorobenzene-d4	8.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	78
2		3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	64
3		Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	53
4		Formic acid, 3,3-dimethylbut-2-yl...	130	C7H14O2	1000368-20-5	39
5		1-Butene, 4-butoxy-	128	C8H16O	034061-76-2	23



Data Path : Z:\HPCHEM1\BNA G\DATA\BG110416\
Data File : BG024706.D
Acq On : 5 Nov 2016 10:47
Operator : UM/SJ
Sample : H5509-24
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GW-94-8.8-20.0

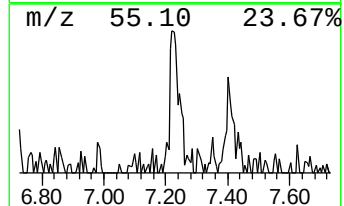
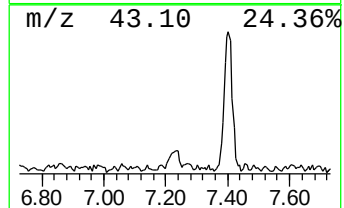
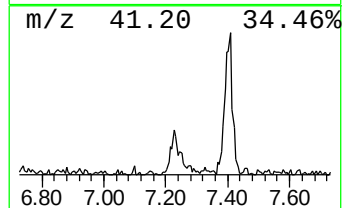
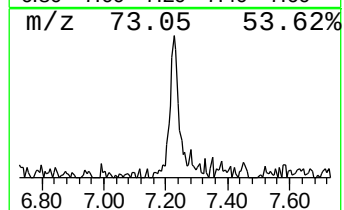
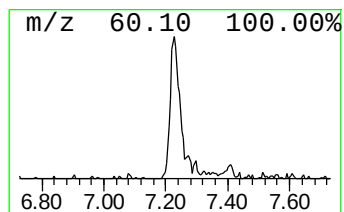
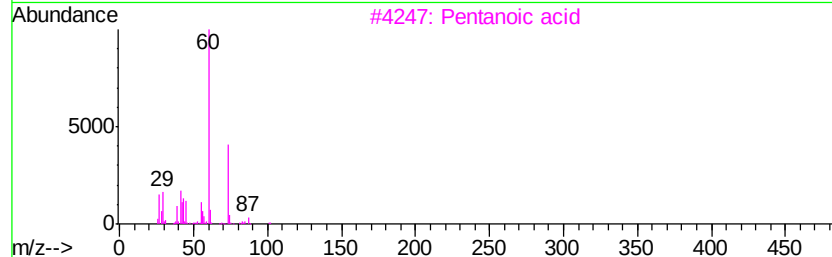
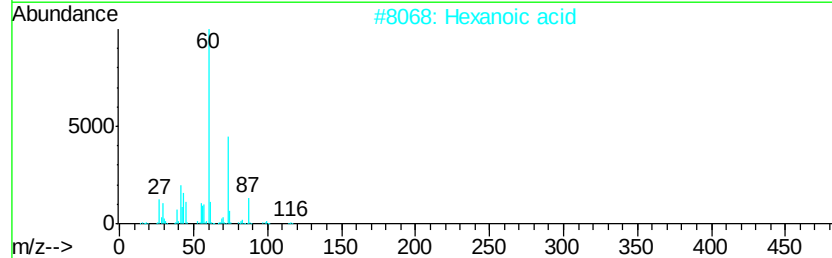
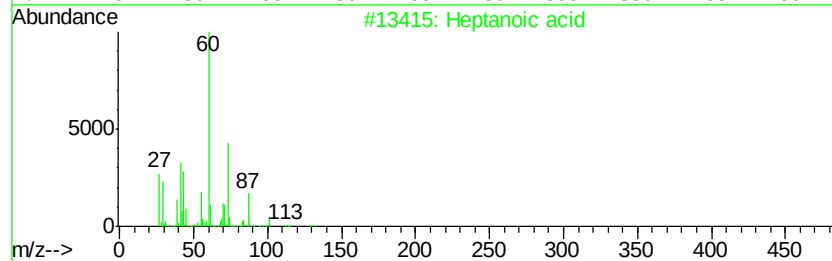
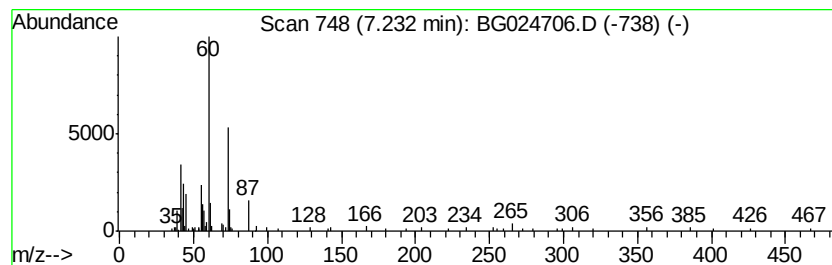
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Heptanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.23	3.93 ng	152932	1,4-Dichlorobenzene-d4	8.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanoic acid	130	C7H14O2	000111-14-8	72
2	Hexanoic acid	116	C6H12O2	000142-62-1	72
3	Pentanoic acid	102	C5H10O2	000109-52-4	64
4	Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	50
5	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	45



Data Path : Z:\HPCHEM1\BNA G\DATA\BG110416\
Data File : BG024706.D
Acq On : 5 Nov 2016 10:47
Operator : UM/SJ
Sample : H5509-24
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GW-94-8.8-20.0

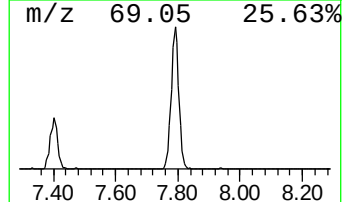
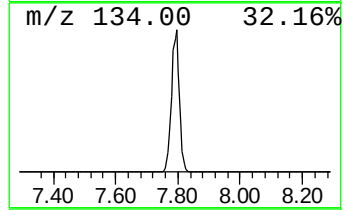
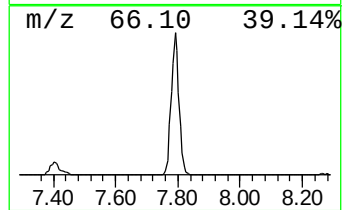
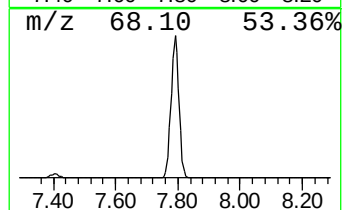
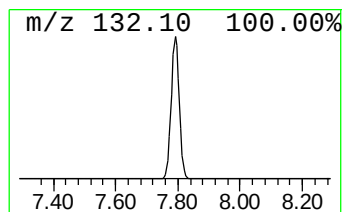
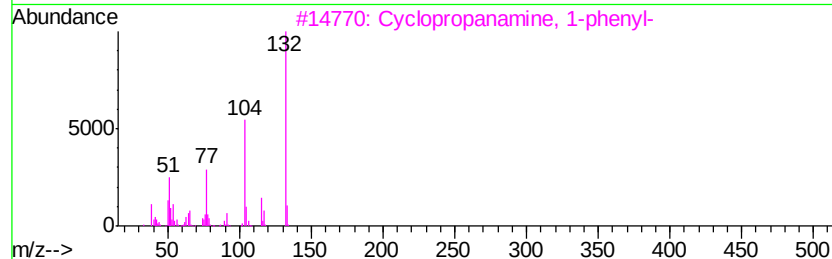
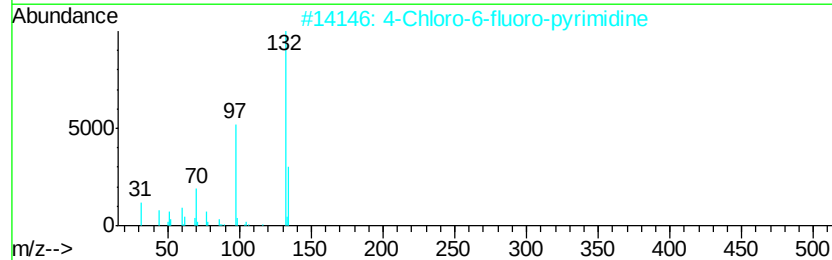
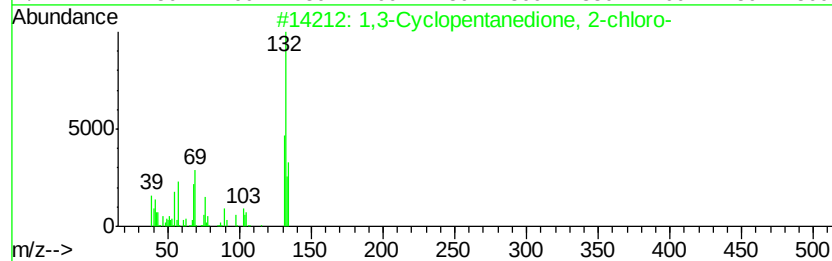
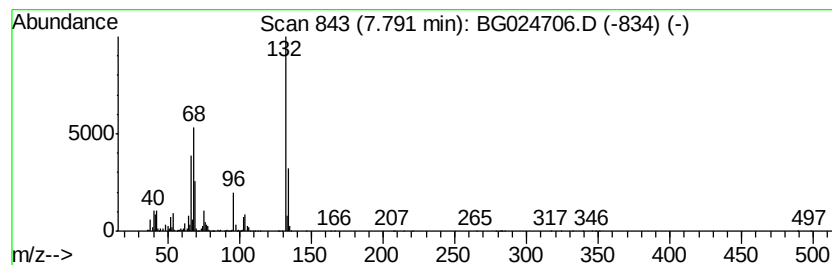
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown7.79 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.79	97.83 ng	3802010	1,4-Dichlorobenzene-d4	8.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	22
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
3		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



Data Path : Z:\HPCHEM1\BNA G\DATA\BG110416\
Data File : BG024706.D
Acq On : 5 Nov 2016 10:47
Operator : UM/SJ
Sample : H5509-24
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GW-94-8.8-20.0

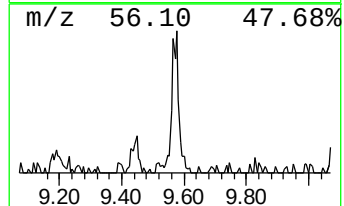
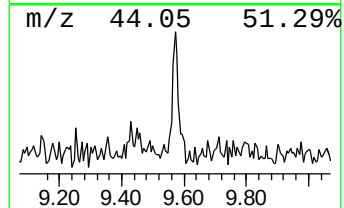
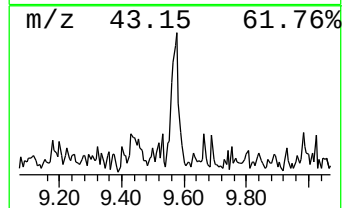
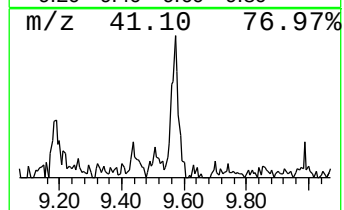
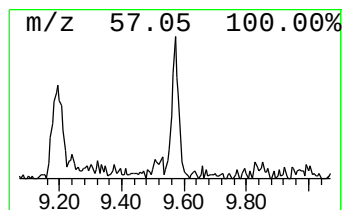
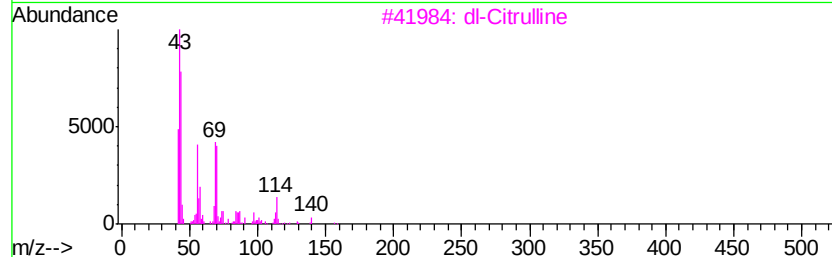
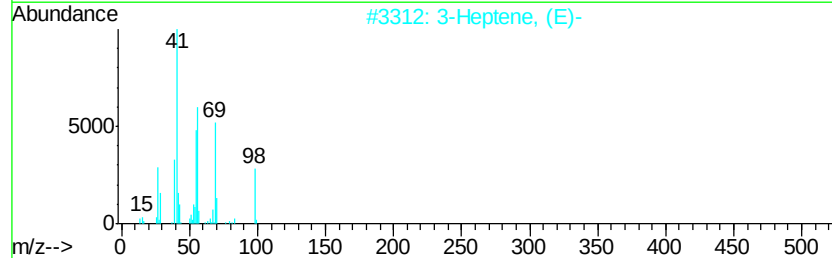
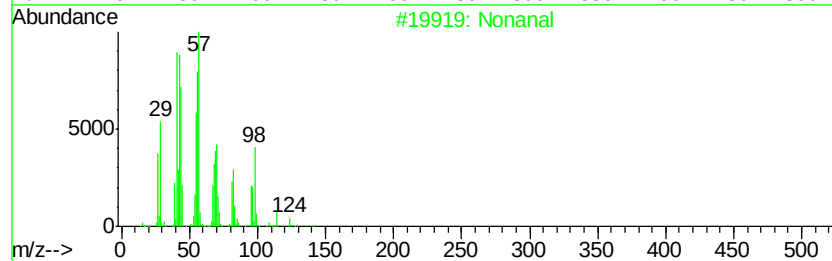
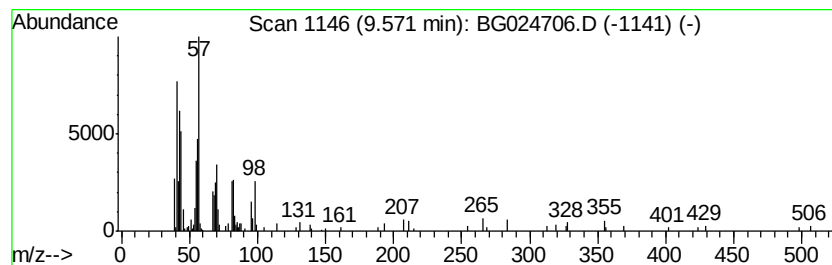
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Nonanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.57	3.44 ng	133556	1,4-Dichlorobenzene-d4	8.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonanal	142	C9H18O	000124-19-6	64
2		3-Heptene, (E)-	98	C7H14	014686-14-7	35
3		dl-Citrulline	175	C6H13N3O3	000627-77-0	35
4		1-Methyl-2-pyrrolidone-4-carboxa...	142	C6H10N2O2	089677-16-7	35
5		Butane, 1-isocyanato-	99	C5H9NO	000111-36-4	35



Data Path : Z:\HPCHEM1\BNA G\DATA\BG110416\
Data File : BG024706.D
Acq On : 5 Nov 2016 10:47
Operator : UM/SJ
Sample : H5509-24
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GW-94-8.8-20.0

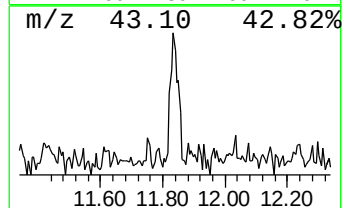
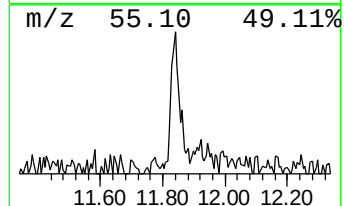
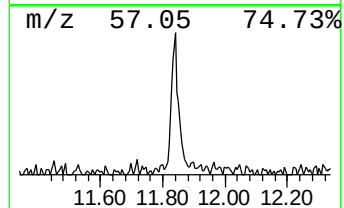
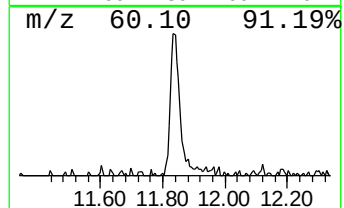
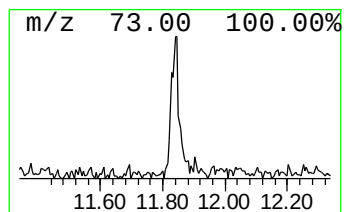
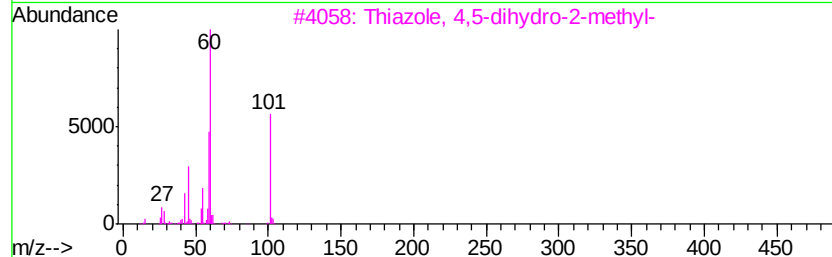
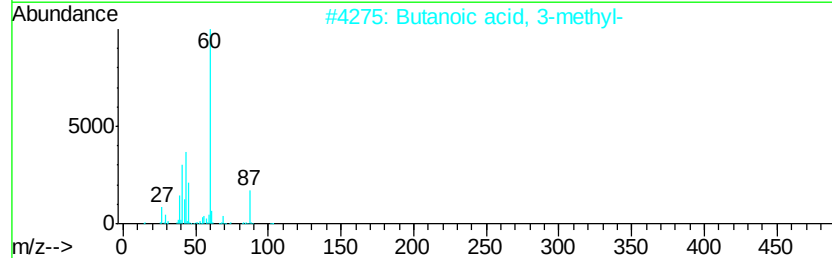
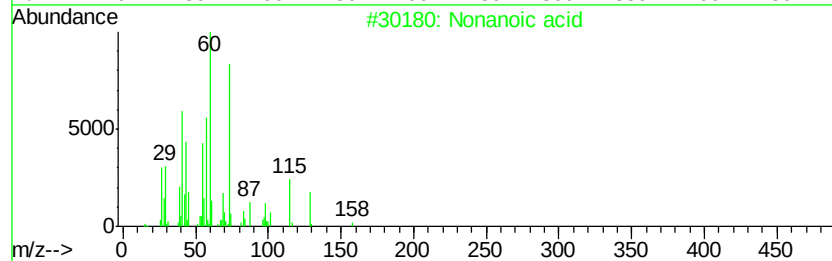
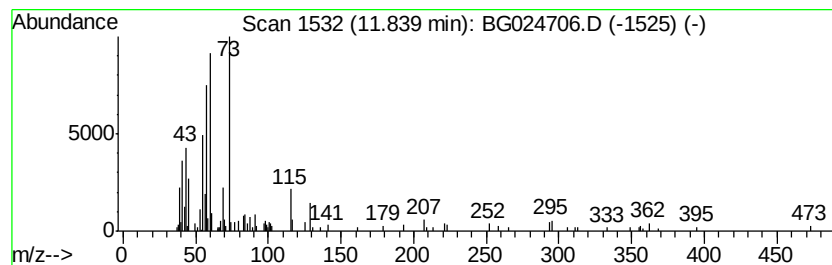
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Nonanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.84	2.55 ng	154161	Napthalene-d8	11.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonanoic acid	158	C9H18O2	000112-05-0	50
2		Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	43
3		Thiazole, 4,5-dihydro-2-methyl-	101	C4H7NS	002346-00-1	43
4		n-Decanoic acid	172	C10H20O2	000334-48-5	42
5		12-Bromododecanoic acid	278	C12H23BrO2	073367-80-3	40



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110416\
Data File : BG024706.D
Acq On : 5 Nov 2016 10:47
Operator : UM/SJ
Sample : H5509-24
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GW-94-8.8-20.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.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
1-Butanol	3.20	3.2	ng	123701	1	8.26	777307	20.0
2-Pentanone, 4-hy...	5.33	8.7	ng	336370	1	8.26	777307	20.0
Ethanol, 2-butoxy-	6.31	179.5	ng	6975210	1	8.26	777307	20.0
Heptanoic acid	7.23	3.9	ng	152932	1	8.26	777307	20.0
unknown7.79	7.79	97.8	ng	3802010	1	8.26	777307	20.0
Nonanal	9.57	3.4	ng	133556	1	8.26	777307	20.0
Nonanoic acid	11.84	2.5	ng	154161	2	11.09	1211410	20.0