

Data Path : Z:\HPCHEM1\BNA G\DATA\BG012518\
 Data File : BG032315.D
 Acq On : 26 Jan 2018 5:24
 Operator : SJ/JU
 Sample : J1267-01
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 IGW-3

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-BG011218.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	3.475	27	32	48	rBV	325058	488964	13.84%	3.027%
2	4.322	171	176	187	rVB	23999	39882	1.13%	0.247%
3	5.009	286	293	305	rVB	215109	353901	10.01%	2.191%
4	5.667	399	405	416	rVB	102195	167723	4.75%	1.038%
5	6.178	485	492	506	rBV	426426	734638	20.79%	4.548%
6	7.859	770	778	791	rVB	410987	753865	21.33%	4.667%
7	8.258	838	846	855	rBV	504608	923174	26.12%	5.716%
8	8.746	921	929	937	rBV	104987	189220	5.35%	1.172%
9	9.081	978	986	994	rBV	508366	924306	26.15%	5.723%
10	9.938	1125	1132	1145	rVB	362043	690190	19.53%	4.273%
11	11.625	1407	1419	1425	rBV2	139371	278975	7.89%	1.727%
12	13.235	1687	1693	1700	rVB	28355	46643	1.32%	0.289%
13	13.452	1724	1730	1740	rBV	23461	39978	1.13%	0.248%
14	13.998	1816	1823	1832	rBV	1403344	2275813	64.39%	14.091%
15	14.797	1954	1959	1963	rBV	28774	44838	1.27%	0.278%
16	15.373	2050	2057	2064	rVB2	266399	440385	12.46%	2.727%
17	16.701	2277	2283	2291	rVB	114925	168863	4.78%	1.046%
18	16.848	2300	2308	2316	rBV	1069739	1789315	50.63%	11.078%
19	18.105	2515	2522	2532	rBV	398352	669452	18.94%	4.145%
20	20.638	2947	2953	2962	rBV	2573390	3534194	100.00%	21.882%
21	22.436	3251	3259	3269	rBV	481398	872706	24.69%	5.403%
22	26.137	3876	3889	3902	rBV3	213822	724343	20.50%	4.485%

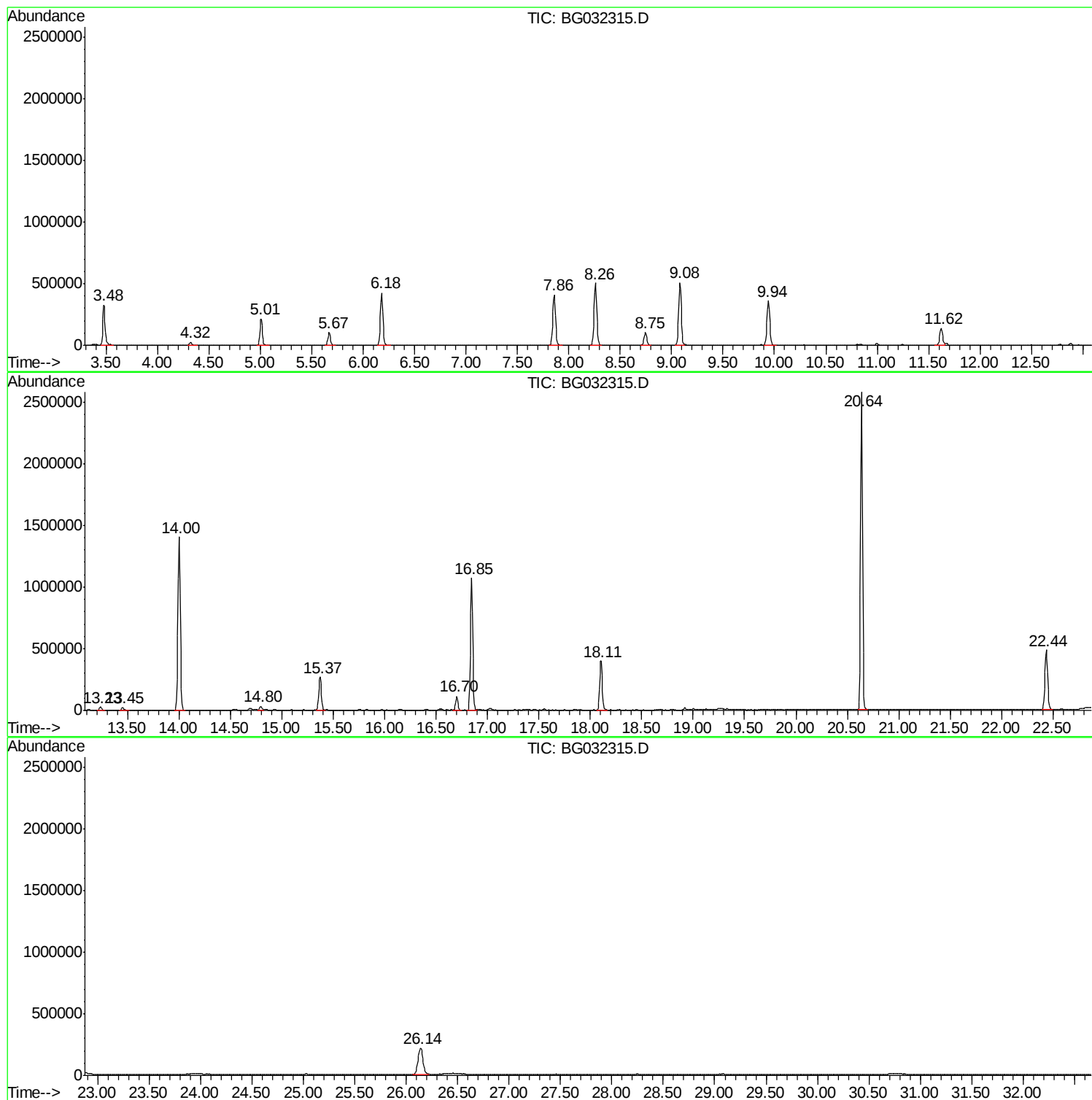
Sum of corrected areas: 16151368

Data Path : Z:\HPCHEM1\BNA G\DATA\BG012518\
Data File : BG032315.D
Acq On : 26 Jan 2018 5:24
Operator : SJ/JU
Sample : J1267-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
IGW-3

Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG011218.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\BG012518\
Data File : BG032315.D
Acq On : 26 Jan 2018 5:24
Operator : SJ/JU
Sample : J1267-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
IGW-3

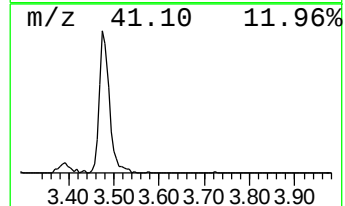
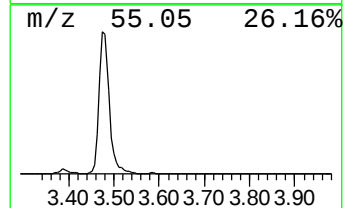
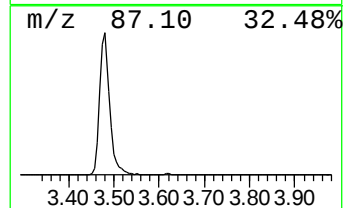
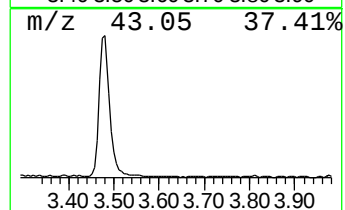
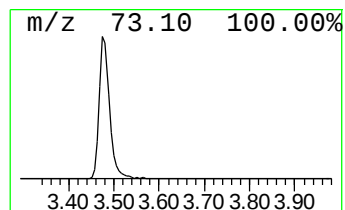
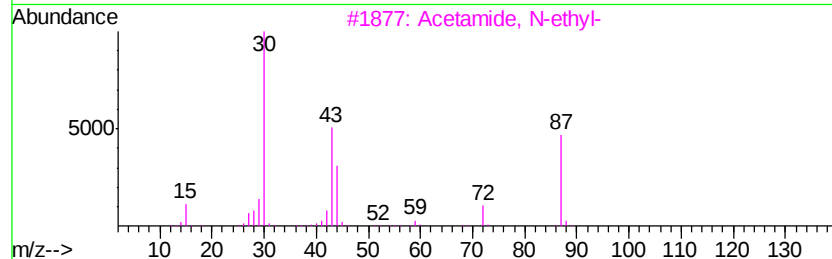
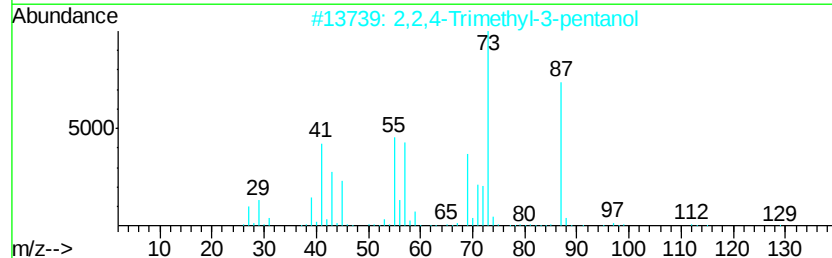
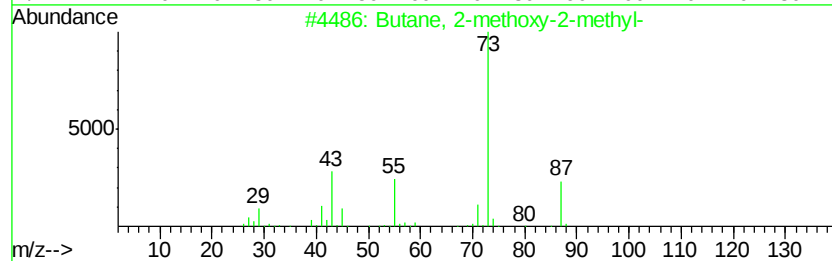
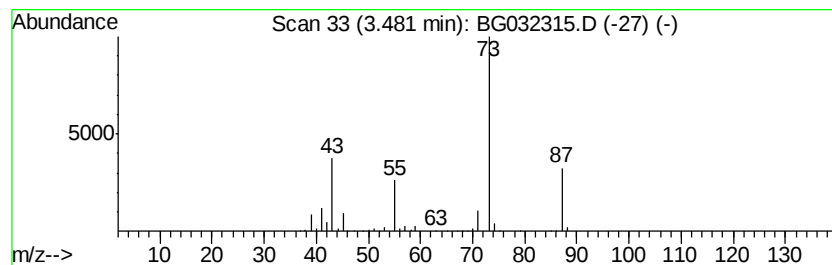
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.48	51.68 ng	488964	1,4-Dichlorobenzene-d4	8.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4		N-Ethylformamide	73	C3H7NO	000627-45-2	9
5		1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	9



Data Path : Z:\HPCHEM1\BNA G\DATA\BG012518\
Data File : BG032315.D
Acq On : 26 Jan 2018 5:24
Operator : SJ/JU
Sample : J1267-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
IGW-3

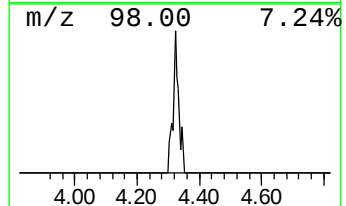
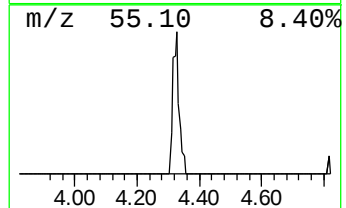
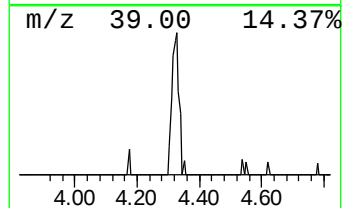
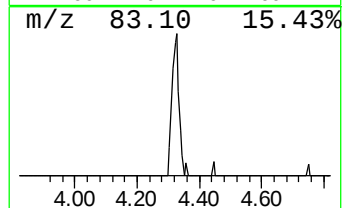
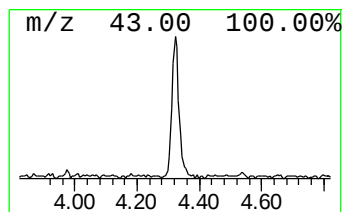
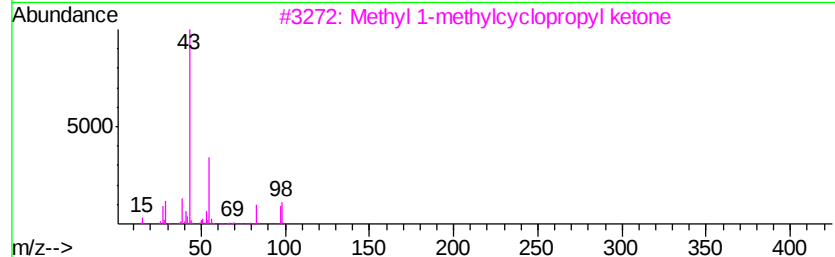
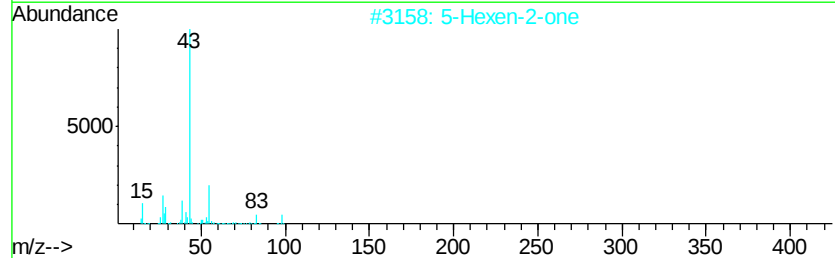
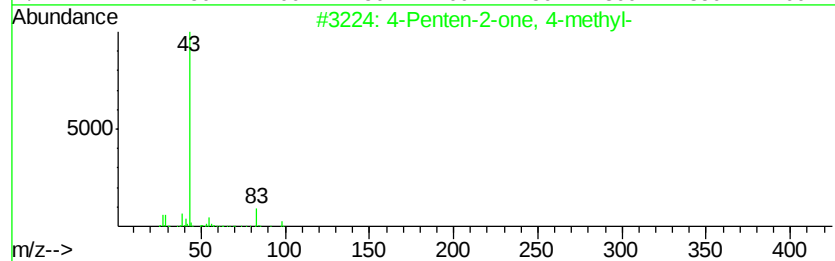
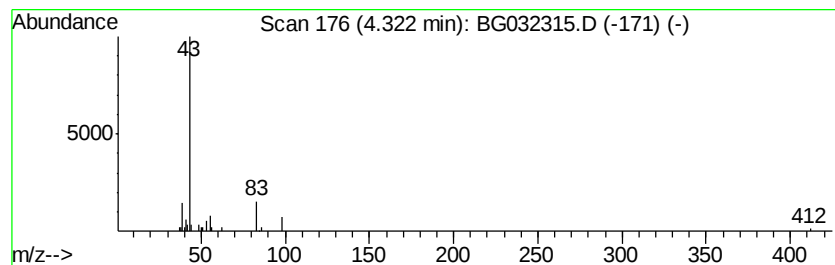
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 4-Penten-2-one, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.32	4.22 ng	39882	1,4-Dichlorobenzene-d4	8.75

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	64
2			5-Hexen-2-one	98	C6H10O	000109-49-9	53
3			Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	47
4			4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	47
5			2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	27



Data Path : Z:\HPCHEM1\BNA G\DATA\BG012518\
Data File : BG032315.D
Acq On : 26 Jan 2018 5:24
Operator : SJ/JU
Sample : J1267-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
IGW-3

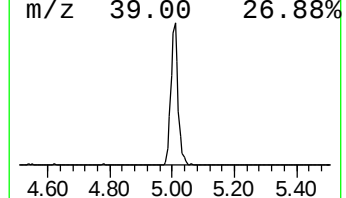
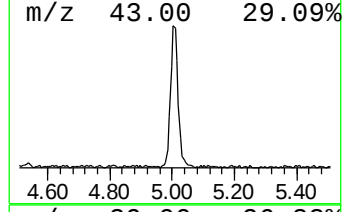
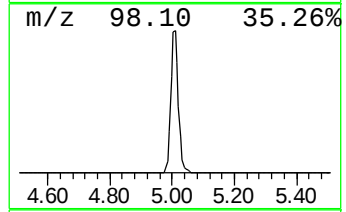
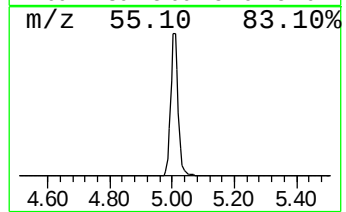
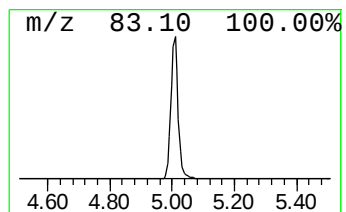
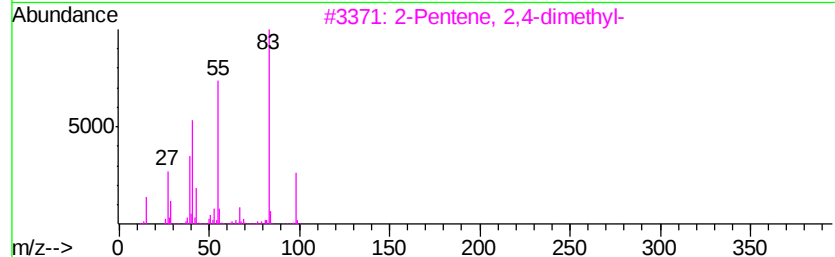
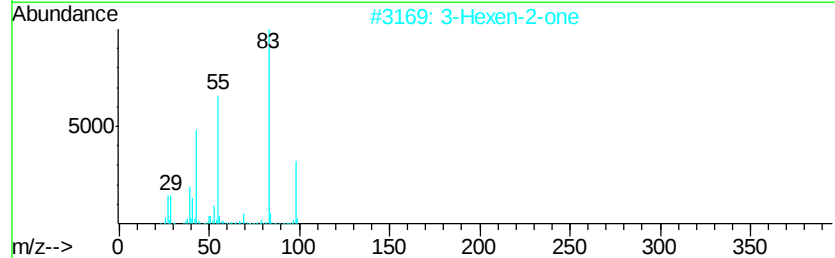
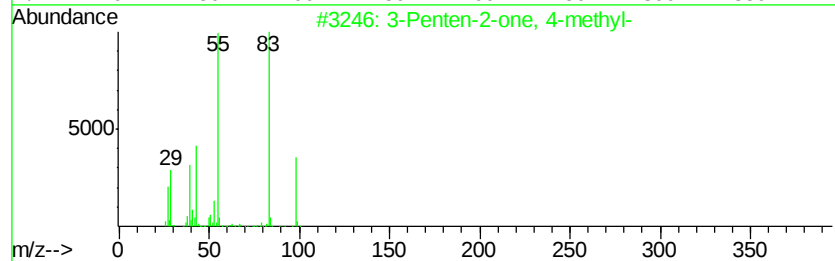
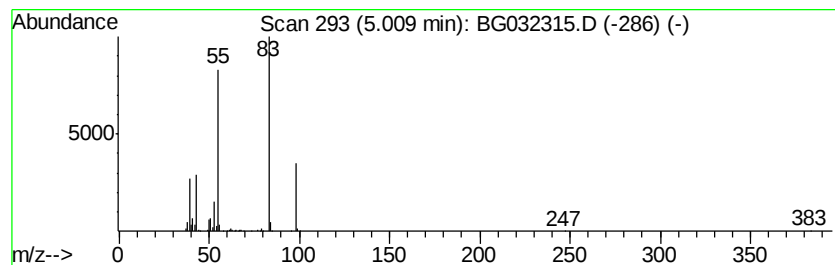
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	37.41 ng	353901	1,4-Dichlorobenzene-d4	8.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	87
2		3-Hexen-2-one	98	C6H10O	000763-93-9	87
3		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
4		Cyclohexane, methyl-	98	C7H14	000108-87-2	80
5		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	78



Data Path : Z:\HPCHEM1\BNA G\DATA\BG012518\
Data File : BG032315.D
Acq On : 26 Jan 2018 5:24
Operator : SJ/JU
Sample : J1267-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
IGW-3

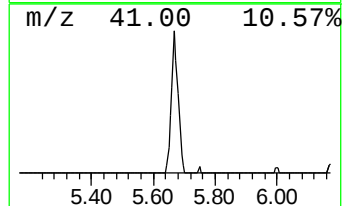
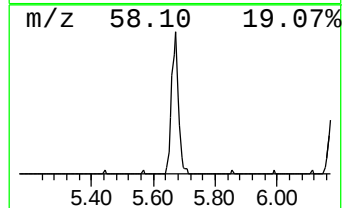
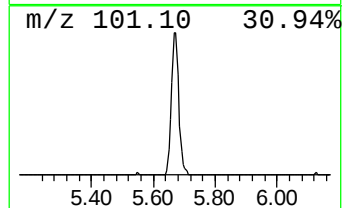
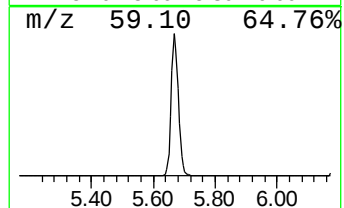
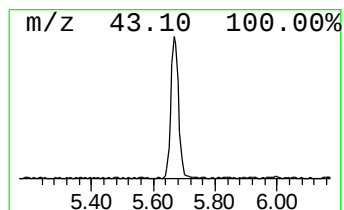
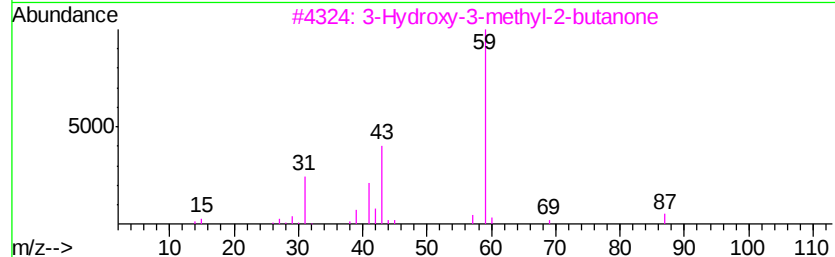
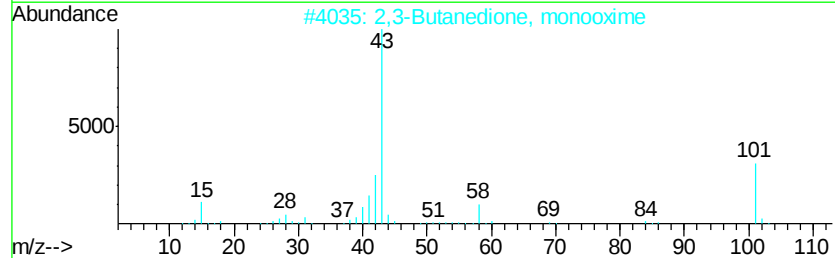
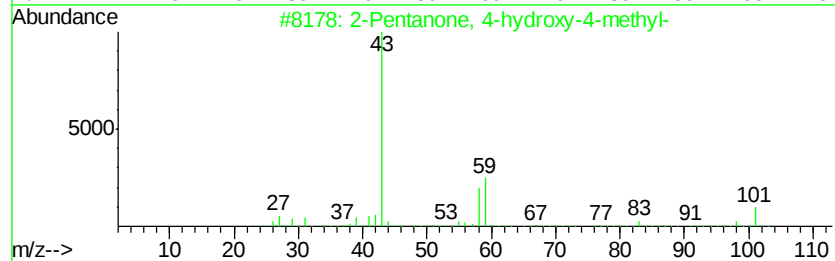
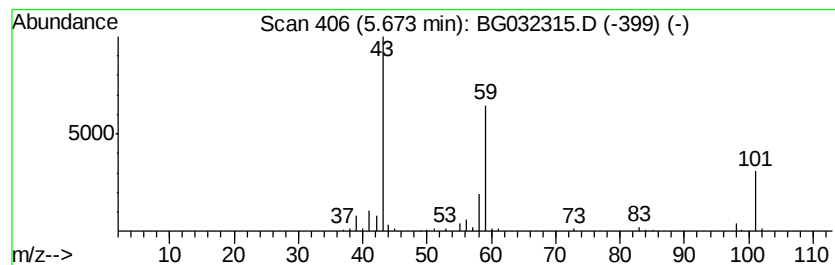
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.67	17.73 ng	167723	1,4-Dichlorobenzene-d4	8.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
3		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	16
4		1-Butanol, 3-methoxy-	104	C5H12O2	002517-43-3	16
5		1-Butene, 4-ethoxy-	100	C6H12O	044611-46-3	12



Data Path : Z:\HPCHEM1\BNA G\DATA\BG012518\
Data File : BG032315.D
Acq On : 26 Jan 2018 5:24
Operator : SJ/JU
Sample : J1267-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
IGW-3

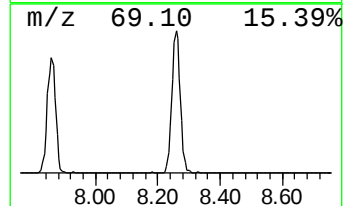
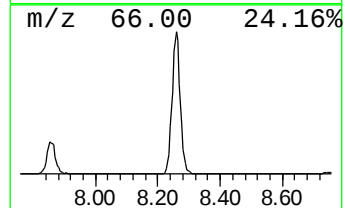
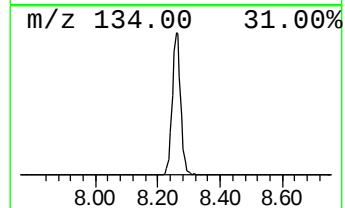
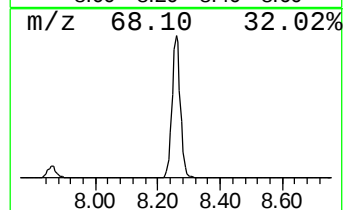
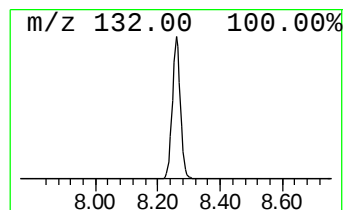
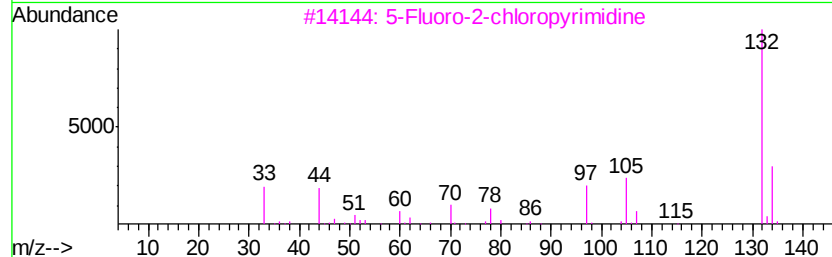
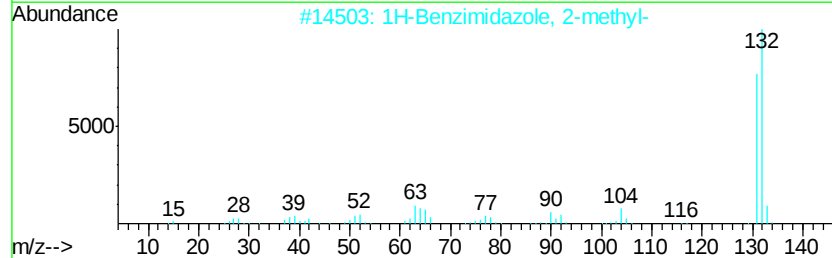
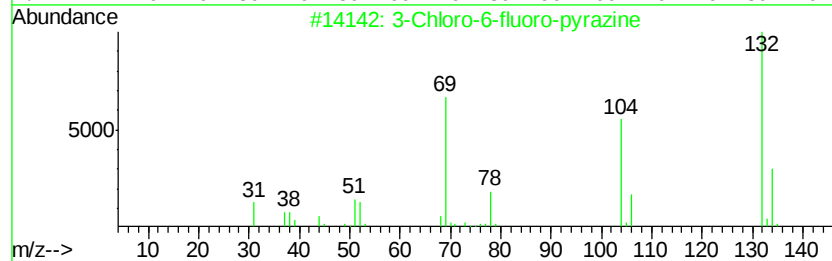
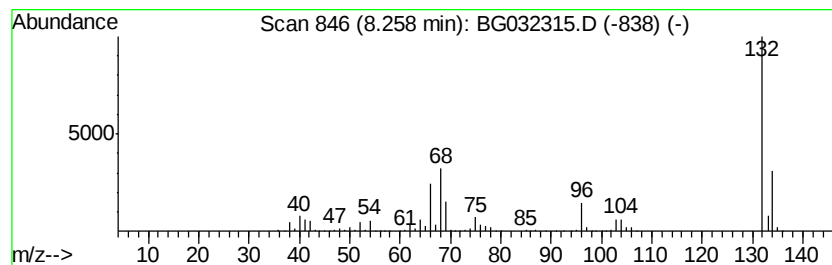
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown8.26 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.26	97.58 ng	923174	1,4-Dichlorobenzene-d4	8.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	27
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	17
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12



Data Path : Z:\HPCHEM1\BNA G\DATA\BG012518\
Data File : BG032315.D
Acq On : 26 Jan 2018 5:24
Operator : SJ/JU
Sample : J1267-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
IGW-3

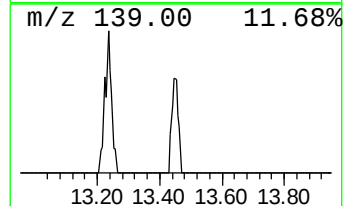
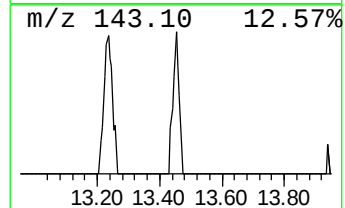
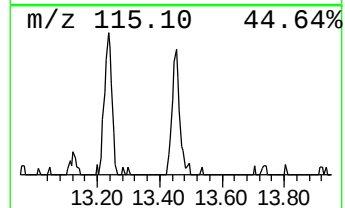
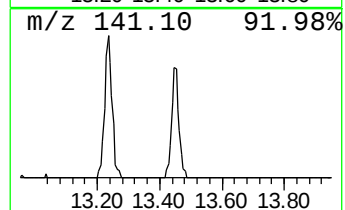
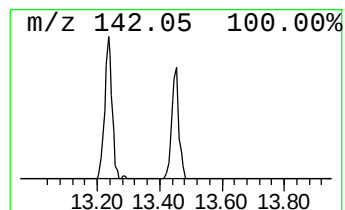
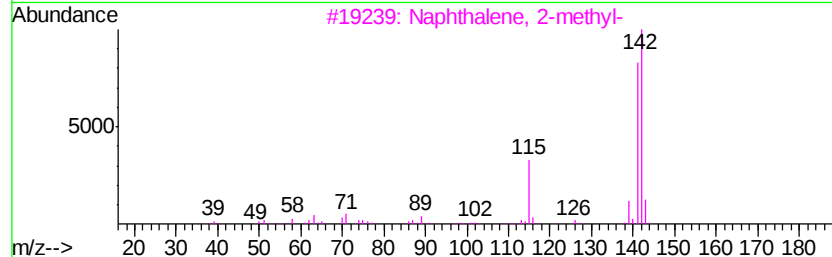
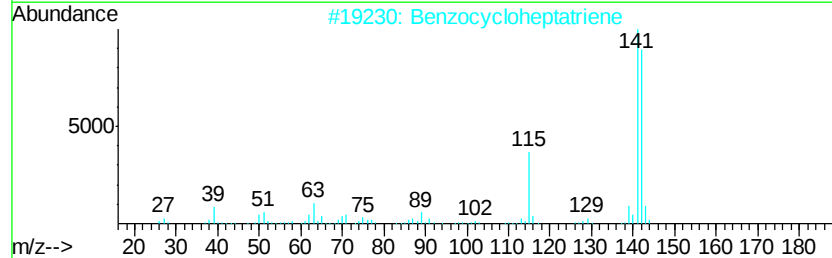
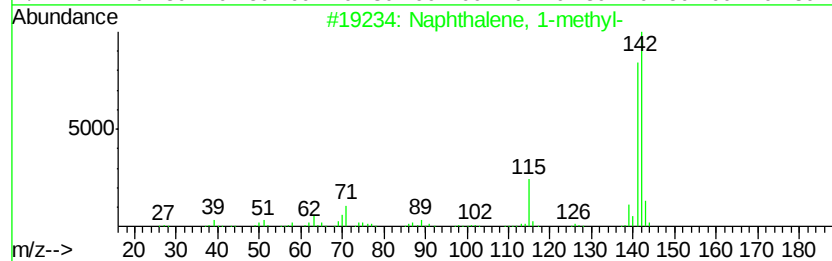
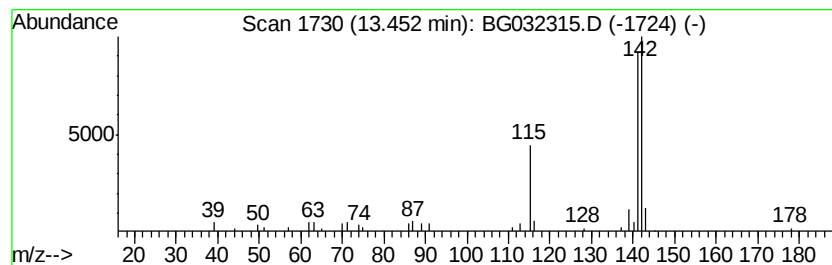
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Naphthalene, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.45	2.87 ng	39978	Naphthalene-d8	11.62

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	91
2			Benzocycloheptatriene	142	C11H10	000264-09-5	91
3			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	91
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	86
5			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	64



Data Path : Z:\HPCHEM1\BNA G\DATA\BG012518\
Data File : BG032315.D
Acq On : 26 Jan 2018 5:24
Operator : SJ/JU
Sample : J1267-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

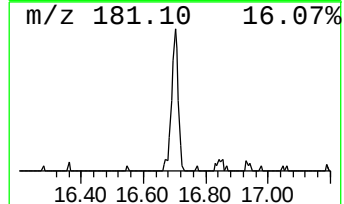
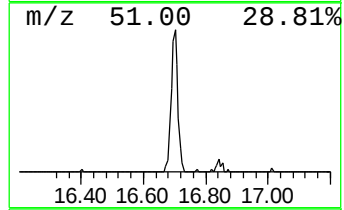
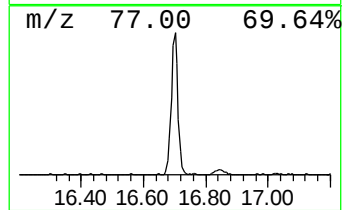
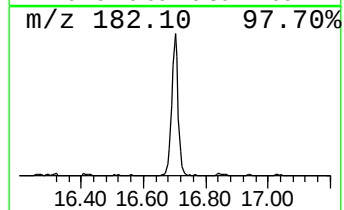
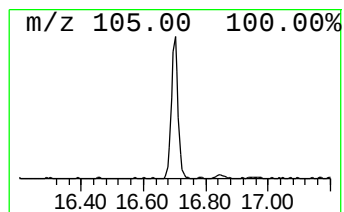
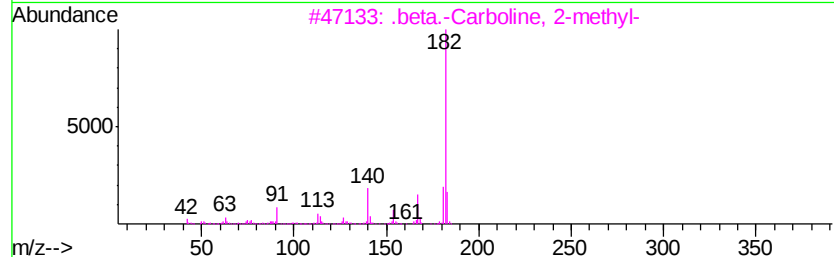
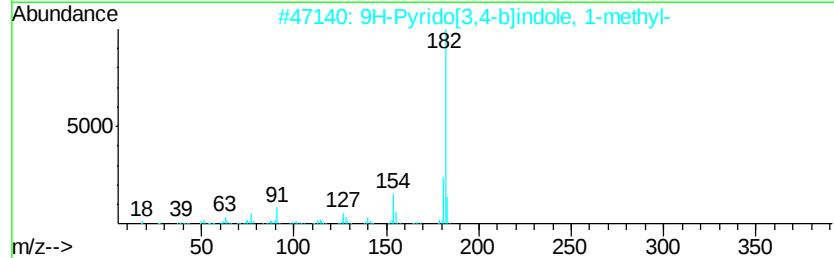
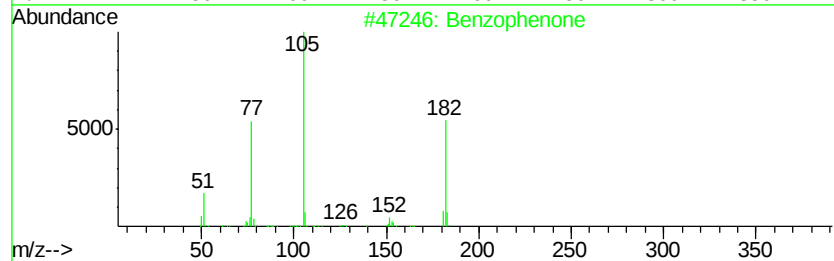
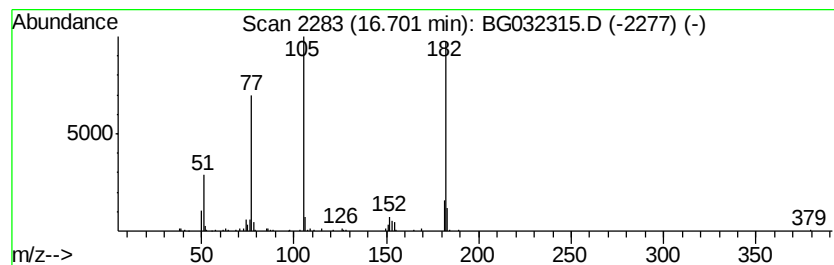
Instrument :
BNA_G
ClientSampleId :
IGW-3

Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
16.70	7.67 ng	168863	Acenaphthene-d10		15.37
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	9H-Pyrido[3,4-b]indole, 1-methyl-	182	C12H10N2	000486-84-0	43
3	.beta.-Carboline, 2-methyl-	182	C12H10N2	013099-99-5	43
4	2,4,6-Trimethoxytoluene	182	C10H14O3	014107-97-2	43
5	Benzoylformic acid	150	C8H6O3	000611-73-4	38



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG012518\
Data File : BG032315.D
Acq On : 26 Jan 2018 5:24
Operator : SJ/JU
Sample : J1267-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
IGW-3

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.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
Butane, 2-methoxy...	3.48	51.7	ng	488964	1	8.75	189220	20.0
4-Penten-2-one, 4...	4.32	4.2	ng	39882	1	8.75	189220	20.0
3-Penten-2-one, 4...	5.01	37.4	ng	353901	1	8.75	189220	20.0
2-Pentanone, 4-hy...	5.67	17.7	ng	167723	1	8.75	189220	20.0
unknown8.26	8.26	97.6	ng	923174	1	8.75	189220	20.0
Naphthalene, 1-me...	13.45	2.9	ng	39978	2	11.62	278975	20.0
Benzophenone	16.70	7.7	ng	168863	3	15.37	440385	20.0