

Data Path : Z:\HPCHEM1\BNA G\DATA\BG101717\
 Data File : BG029315.D
 Acq On : 18 Oct 2017 00:10
 Operator : SJ/JU
 Sample : I5867-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 101117-TIFR-E-U-B

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-BG101617.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	5.244	326	333	341	rBV	55277	88495	1.64%	0.394%
2	5.720	407	414	424	rBV	382620	610741	11.33%	2.723%
3	7.318	678	686	696	rBV	256784	451802	8.38%	2.014%
4	7.700	743	751	759	rBV	684764	1199088	22.25%	5.345%
5	8.170	824	831	837	rBV	227634	384844	7.14%	1.716%
6	8.493	878	886	897	rBV	878115	1561780	28.98%	6.962%
7	9.334	1018	1029	1042	rBV	751228	1373992	25.49%	6.125%
8	10.985	1300	1310	1319	rBV	346649	640085	11.88%	2.853%
9	13.417	1716	1724	1735	rBV	2269712	3636547	67.48%	16.211%
10	14.228	1857	1862	1867	rVB	41333	57057	1.06%	0.254%
11	14.786	1949	1957	1965	rBV2	615299	1026757	19.05%	4.577%
12	16.061	2169	2174	2179	rBV	73044	95145	1.77%	0.424%
13	16.267	2200	2209	2230	rBV	1170044	1871913	34.73%	8.345%
14	17.524	2414	2423	2429	rBV2	791211	1199555	22.26%	5.347%
15	20.115	2858	2864	2870	rBV	4090677	5389285	100.00%	24.024%
16	21.796	3143	3150	3158	rBV2	837319	1401713	26.01%	6.249%
17	23.165	3377	3383	3393	rBV3	40107	111902	2.08%	0.499%
18	25.103	3702	3713	3726	rBV2	414562	1331873	24.71%	5.937%

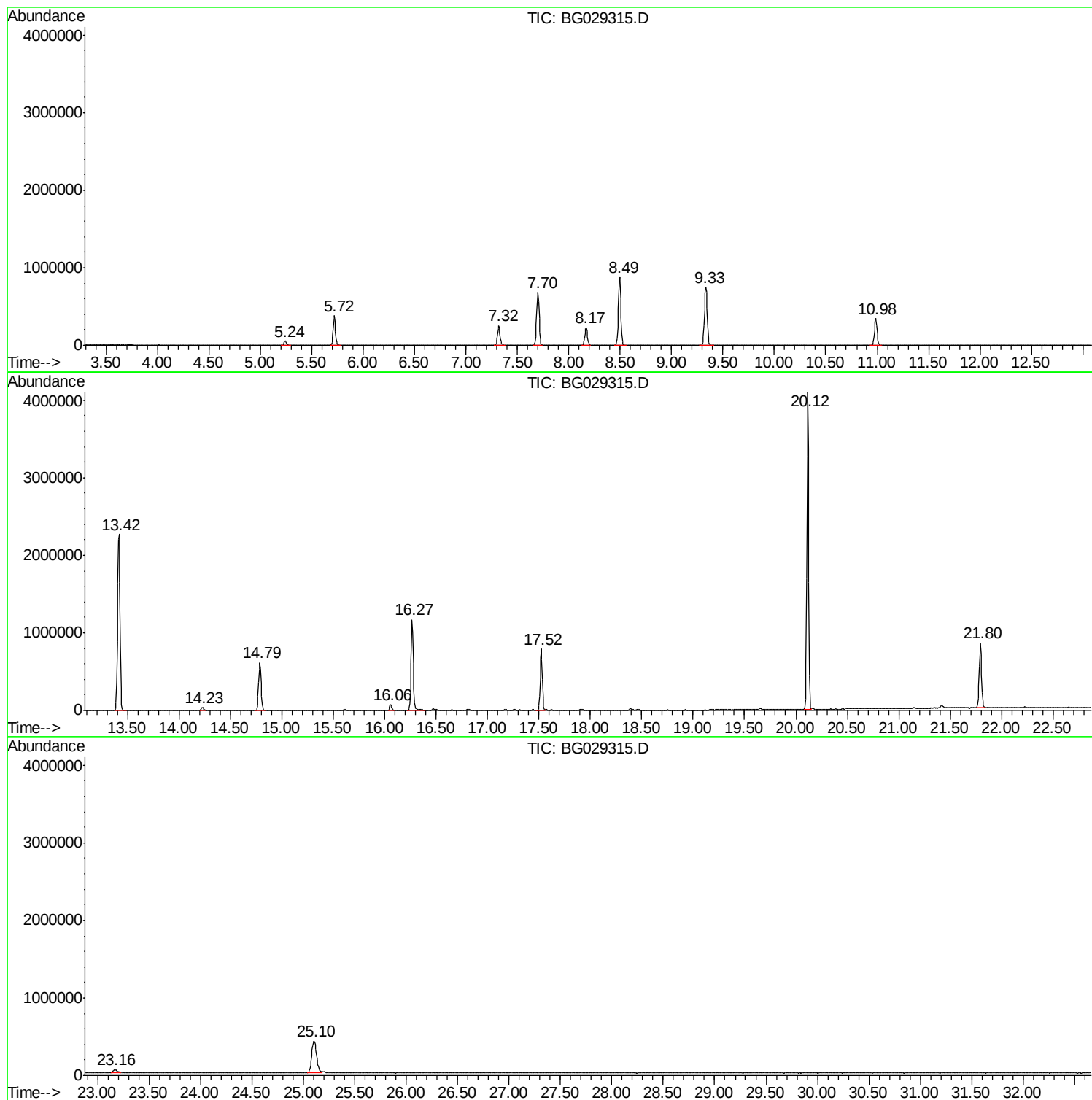
Sum of corrected areas: 22432574

Data Path : Z:\HPCHEM1\BNA G\DATA\BG101717\
Data File : BG029315.D
Acq On : 18 Oct 2017 00:10
Operator : SJ/JU
Sample : I5867-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
101117-TIFR-E-U-B

Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG101617.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\BG101717\
Data File : BG029315.D
Acq On : 18 Oct 2017 00:10
Operator : SJ/JU
Sample : I5867-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
101117-TIFR-E-U-B

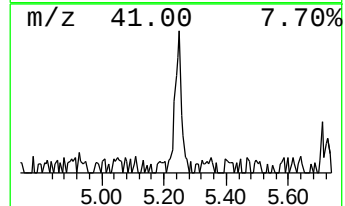
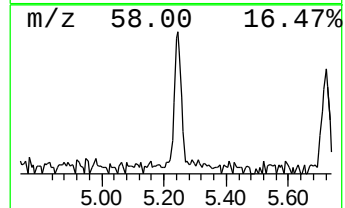
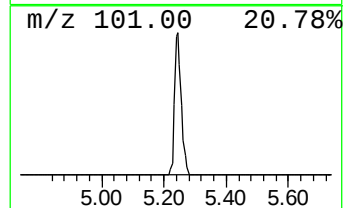
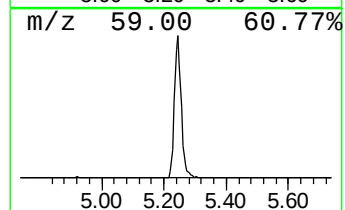
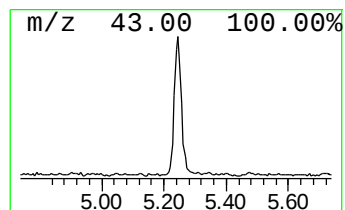
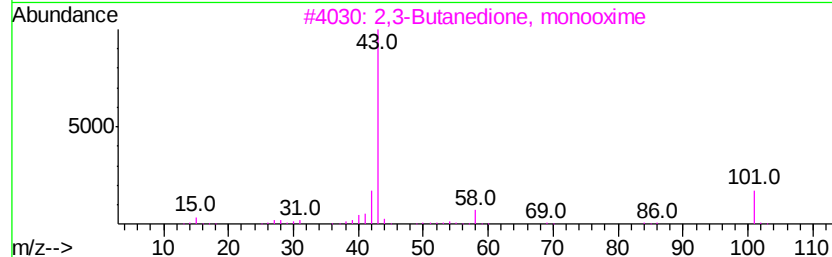
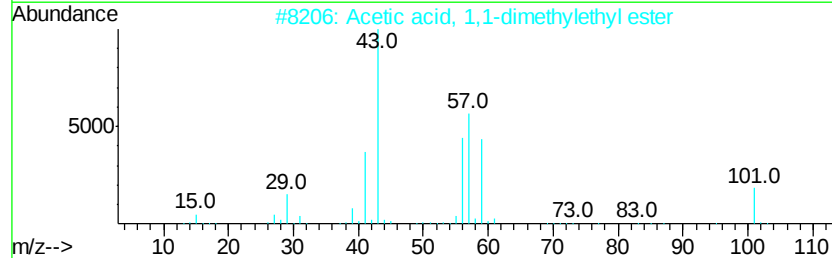
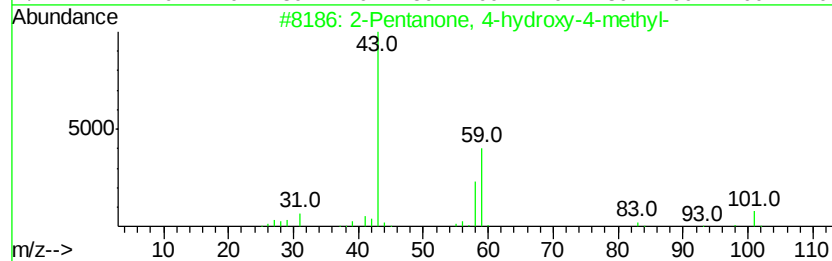
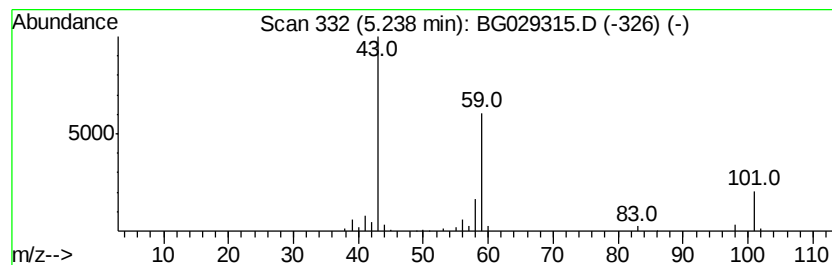
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG101617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.24	4.60 ng	88495	1,4-Dichlorobenzene-d4	8.17

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4			1,2-Butanediol	90	C4H10O2	000584-03-2	23
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17



Data Path : Z:\HPCHEM1\BNA G\DATA\BG101717\
Data File : BG029315.D
Acq On : 18 Oct 2017 00:10
Operator : SJ/JU
Sample : I5867-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
101117-TIFR-E-U-B

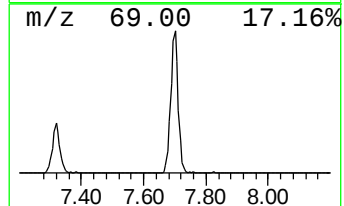
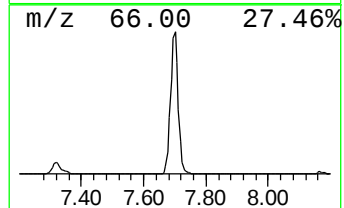
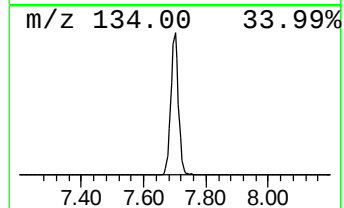
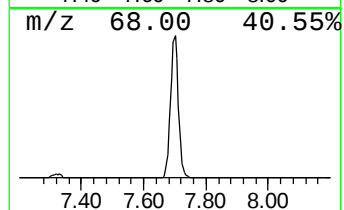
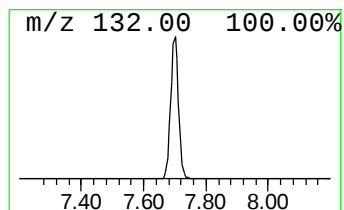
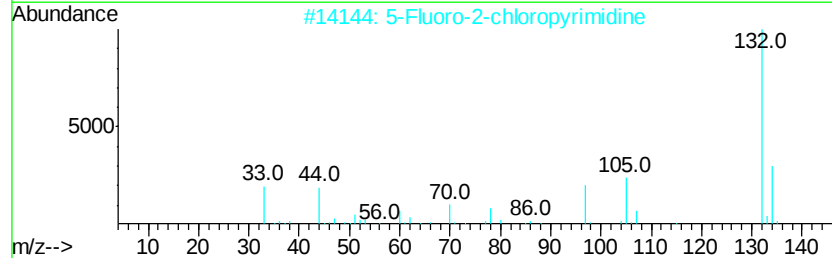
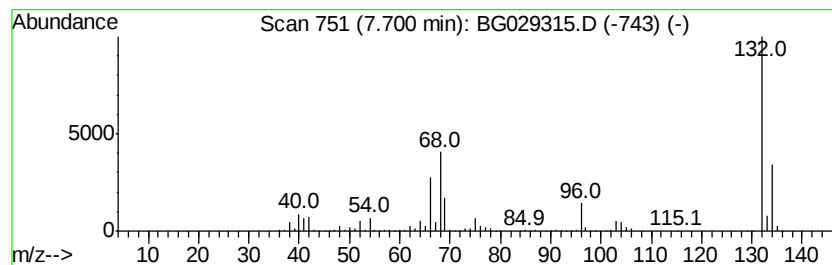
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG101617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown7.70 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.70	62.32 ng	1199090	1,4-Dichlorobenzene-d4	8.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG101717\
Data File : BG029315.D
Acq On : 18 Oct 2017 00:10
Operator : SJ/JU
Sample : I5867-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
101117-TIFR-E-U-B

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101617.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
2-Pentanone, 4-hy...	5.24	4.6	ng	88495	1	8.17	384844	20.0
unknown7.70	7.70	62.3	ng	1199090	1	8.17	384844	20.0