

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041917\
 Data File : BG026656.D
 Acq On : 19 Apr 2017 14:25
 Operator : SJ/MA
 Sample : PB98333BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PB98333BL

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-BG041817.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	4.528	239	245	256	rBV	347734	529790	4.38%	1.135%
2	5.127	339	347	359	rBV	766913	1175080	9.72%	2.518%
3	5.597	421	427	445	rBV	1387064	2280369	18.86%	4.887%
4	7.189	690	698	716	rBV	1304624	2240984	18.53%	4.803%
5	7.560	754	761	779	rBV	1431026	2458683	20.33%	5.269%
6	8.030	832	841	849	rBV	445500	780032	6.45%	1.672%
7	8.353	887	896	905	rBV	1699441	2932949	24.25%	6.285%
8	9.181	1030	1037	1049	rBV	1125732	2051519	16.97%	4.396%
9	10.826	1309	1317	1333	rBV	600741	1122966	9.29%	2.407%
10	13.265	1724	1732	1744	rBV	3583676	5667071	46.86%	12.145%
11	14.634	1958	1965	1979	rBV2	908568	1556581	12.87%	3.336%
12	16.114	2210	2217	2236	rBV	1952457	3159645	26.13%	6.771%
13	17.366	2423	2430	2443	rBV2	1414294	2239546	18.52%	4.799%
14	19.968	2866	2873	2882	rBV	8775088	12092404	100.00%	25.914%
15	21.614	3146	3153	3163	rBV	1994422	3333252	27.56%	7.143%
16	24.786	3681	3693	3707	rBV2	979498	3041977	25.16%	6.519%

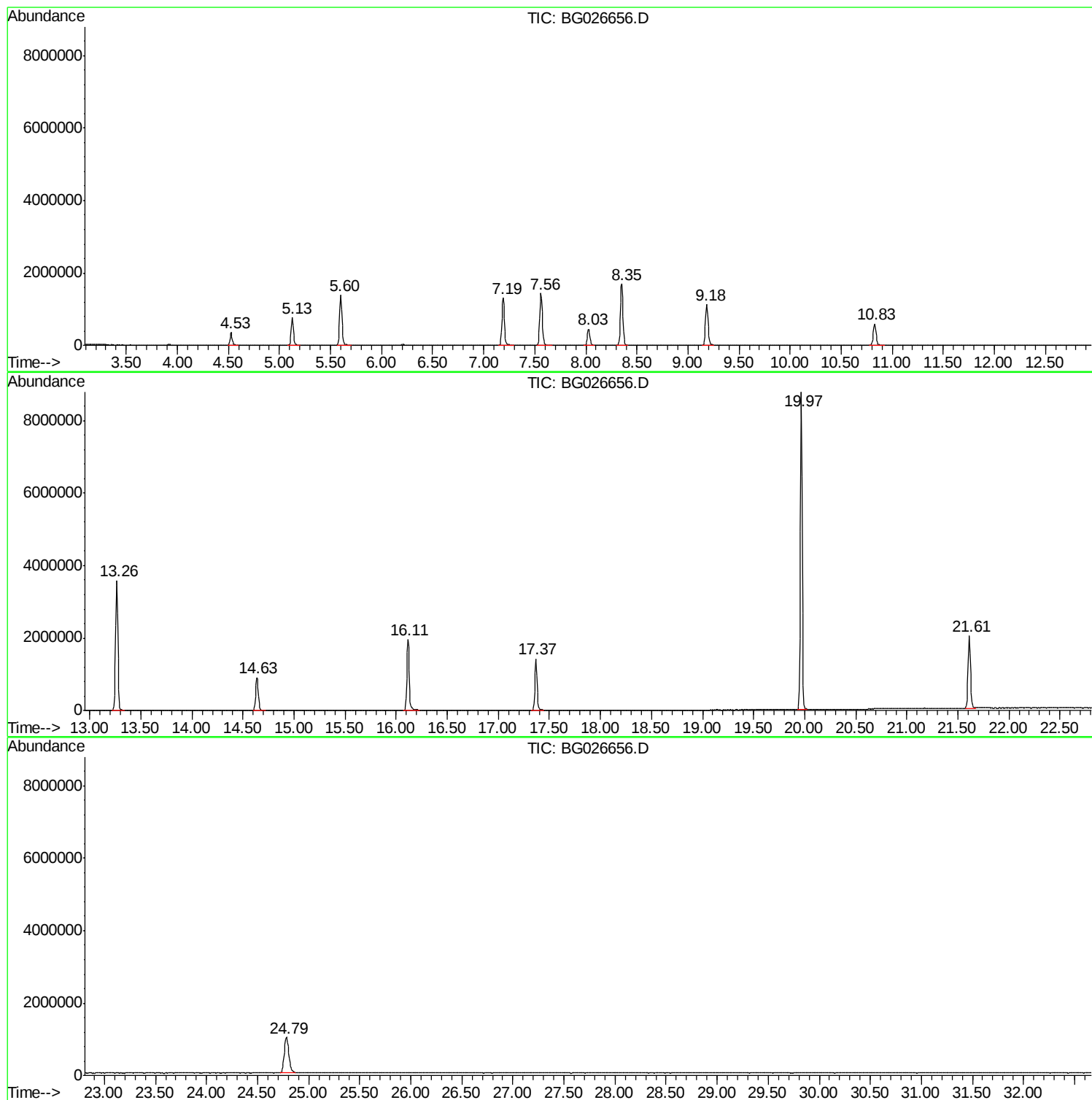
Sum of corrected areas: 46662848

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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG041817.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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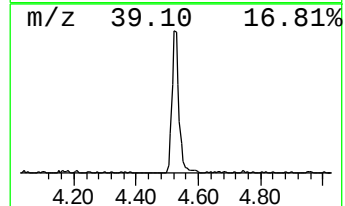
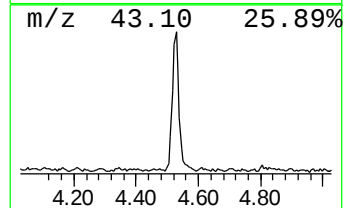
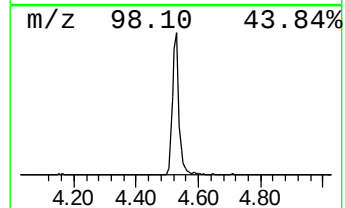
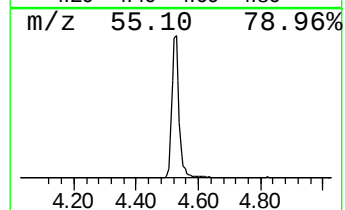
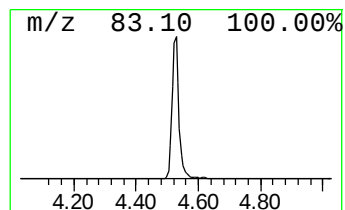
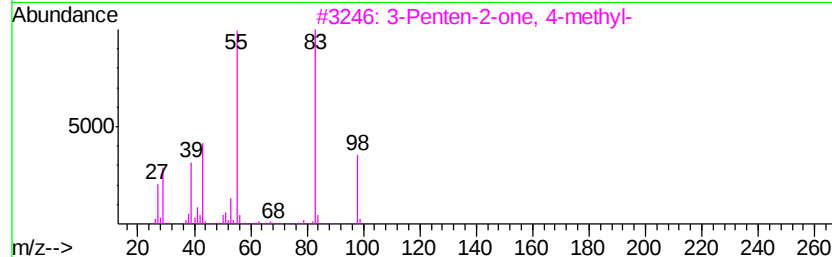
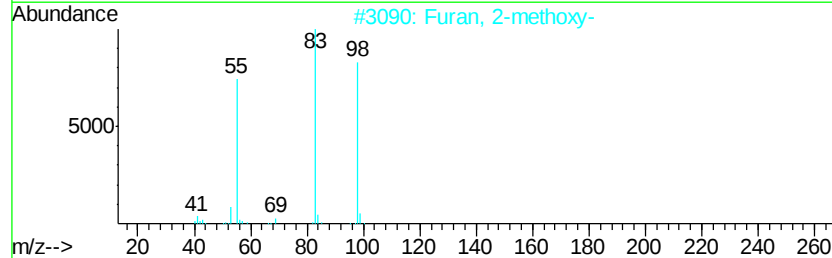
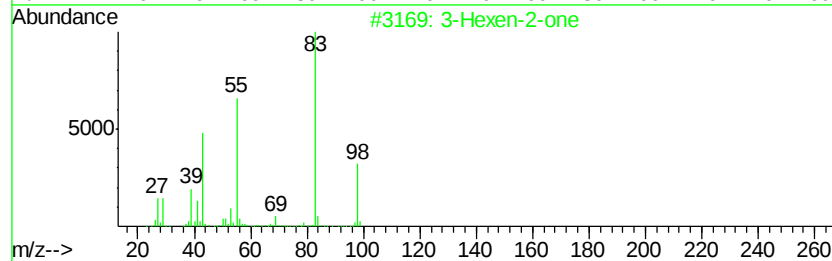
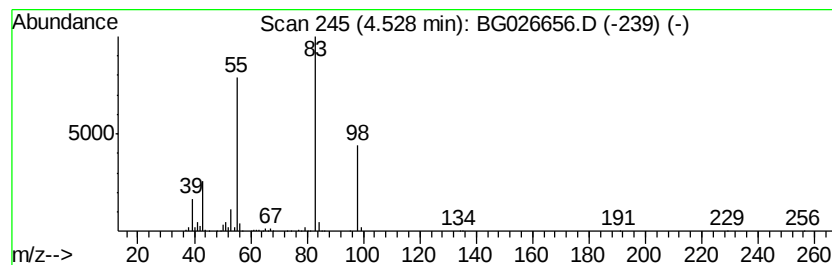
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG041817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Hexen-2-one Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.53	13.58 ng	529790	1,4-Dichlorobenzene-d4	8.03

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hexen-2-one	98	C6H10O	000763-93-9	90
2			Furan, 2-methoxy-	98	C5H6O2	025414-22-6	83
3			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	83
4			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	64
5			2,4-Azetidinedione, 3,3-diethyl-	141	C7H11N2O2	042282-85-9	64



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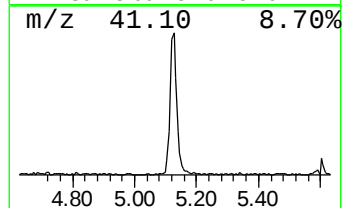
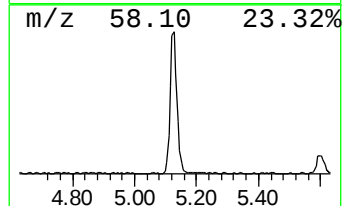
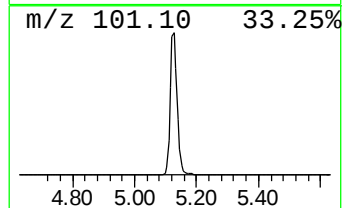
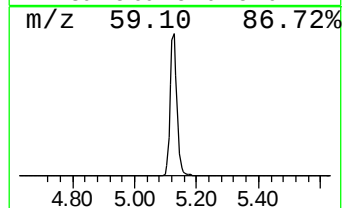
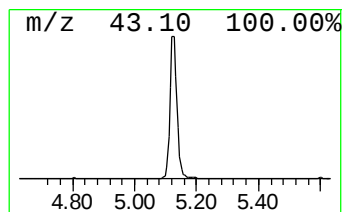
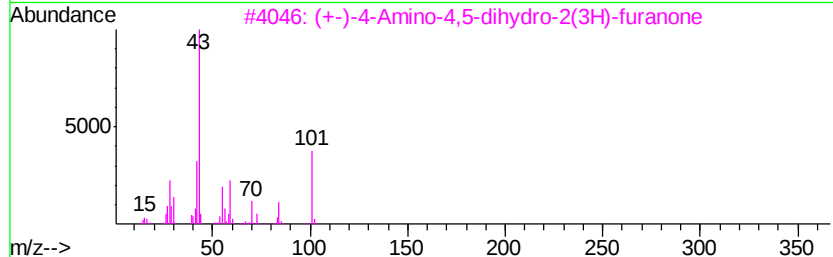
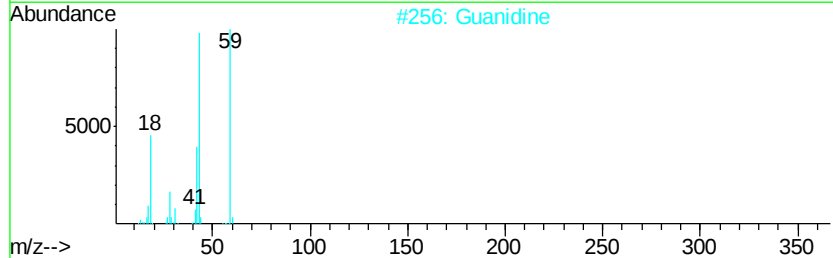
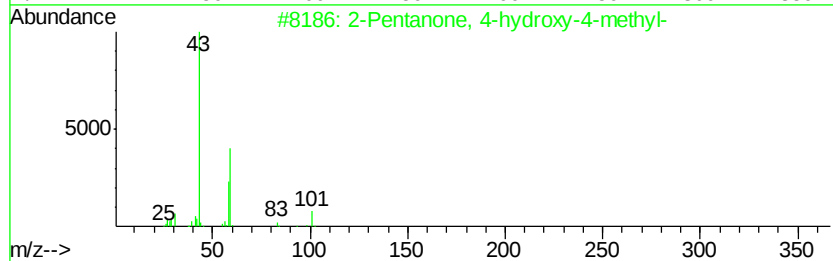
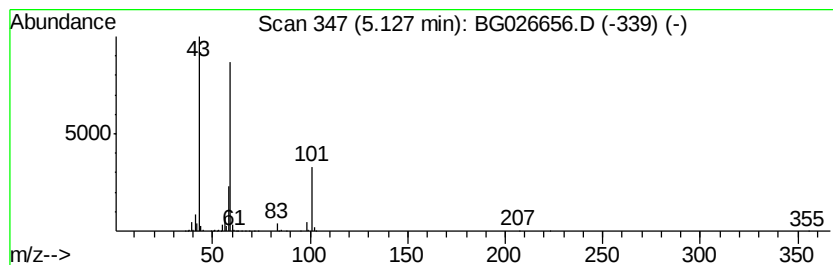
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	30.13 ng	1175080	1,4-Dichlorobenzene-d4	8.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Guanidine	59	CH5N3	000113-00-8	47
3		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	27
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	9



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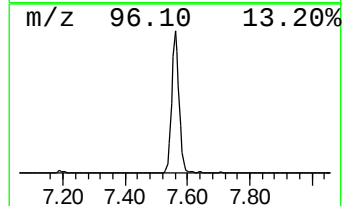
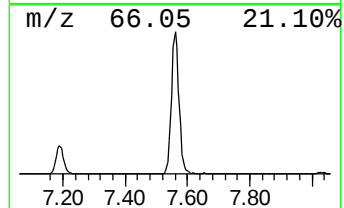
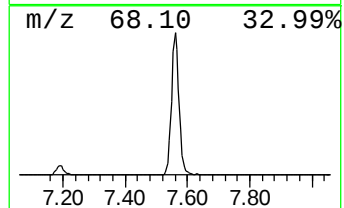
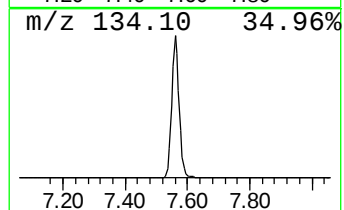
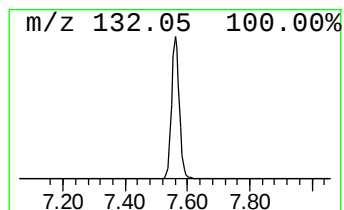
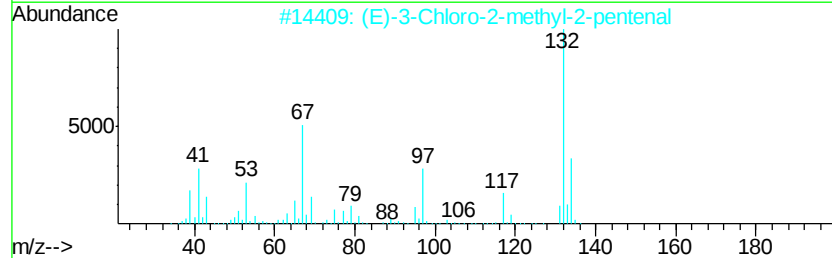
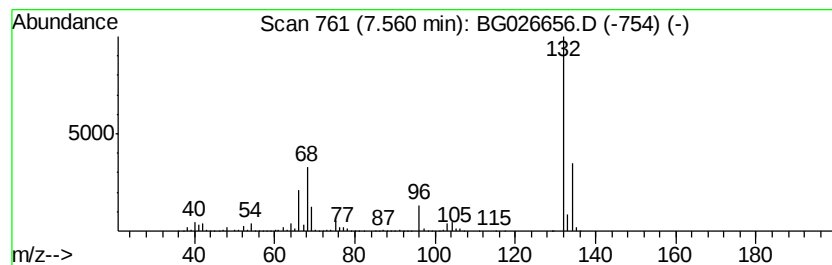
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Peak Number 3 unknown7.56 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.56	63.04 ng	2458680	1,4-Dichlorobenzene-d4	8.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	10
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Hexen-2-one	4.53	13.6	ng	529790	1	8.03	780032	20.0
2-Pentanone, 4-hy...	5.13	30.1	ng	1175080	1	8.03	780032	20.0
unknown7.56	7.56	63.0	ng	2458680	1	8.03	780032	20.0