

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060823\
 Data File : BG057676.D
 Acq On : 8 Jun 2023 18:40
 Operator : CG/JU
 Sample : PB153189BL
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PB153189BL

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:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057676.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.713	271	276	283	rBB	28760	40715	7.36%	2.009%
2	5.341	377	383	393	rBV	147150	230273	41.62%	11.360%
3	5.835	461	467	478	rBB	75493	122615	22.16%	6.049%
4	6.446	566	571	577	rBB2	5901	8577	1.55%	0.423%
5	7.462	738	744	757	rBB2	77529	136790	24.72%	6.748%
6	8.308	883	888	894	rBB2	17885	29963	5.42%	1.478%
7	9.495	1083	1090	1101	rBB	74820	133447	24.12%	6.583%
8	11.146	1365	1371	1380	rBB	24372	41080	7.42%	2.027%
9	13.555	1774	1781	1790	rBB	185260	272058	49.17%	13.421%
10	14.930	2009	2015	2022	rBB2	37641	55449	10.02%	2.735%
11	16.417	2262	2268	2276	rBV	93984	143564	25.95%	7.082%
12	17.668	2474	2481	2487	rBV	52517	79334	14.34%	3.914%
13	20.241	2913	2919	2924	rBV	425733	553278	100.00%	27.294%
14	21.963	3205	3212	3220	rBV2	55784	92511	16.72%	4.564%
15	25.430	3789	3802	3814	rBV2	30919	87441	15.80%	4.314%

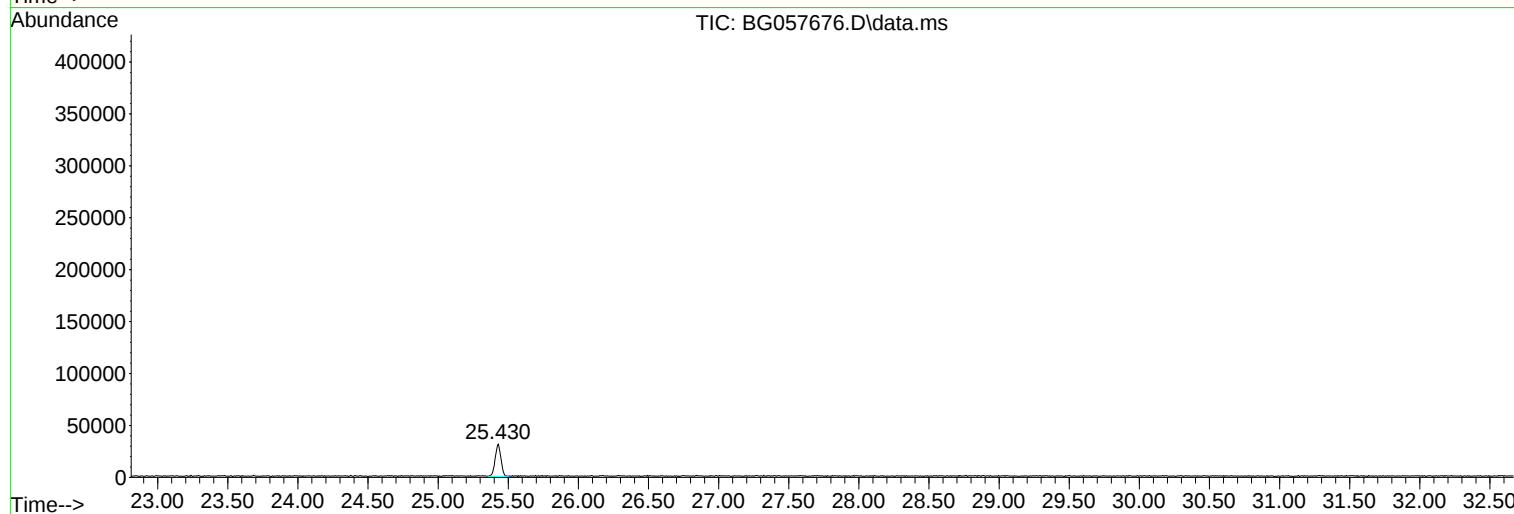
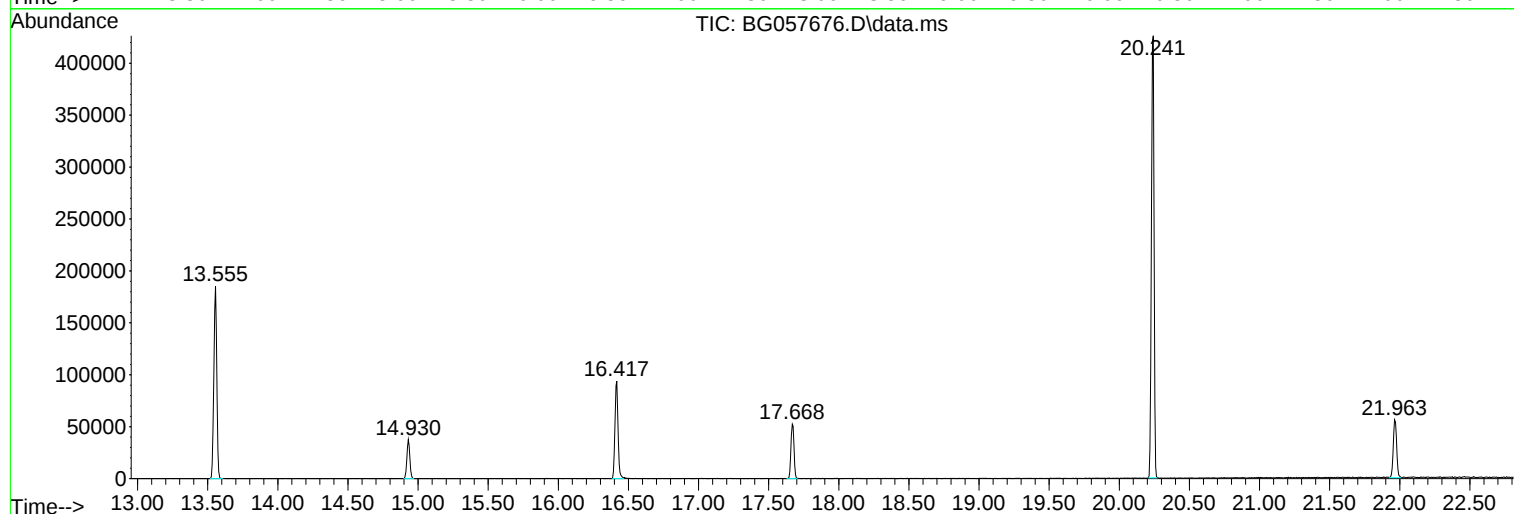
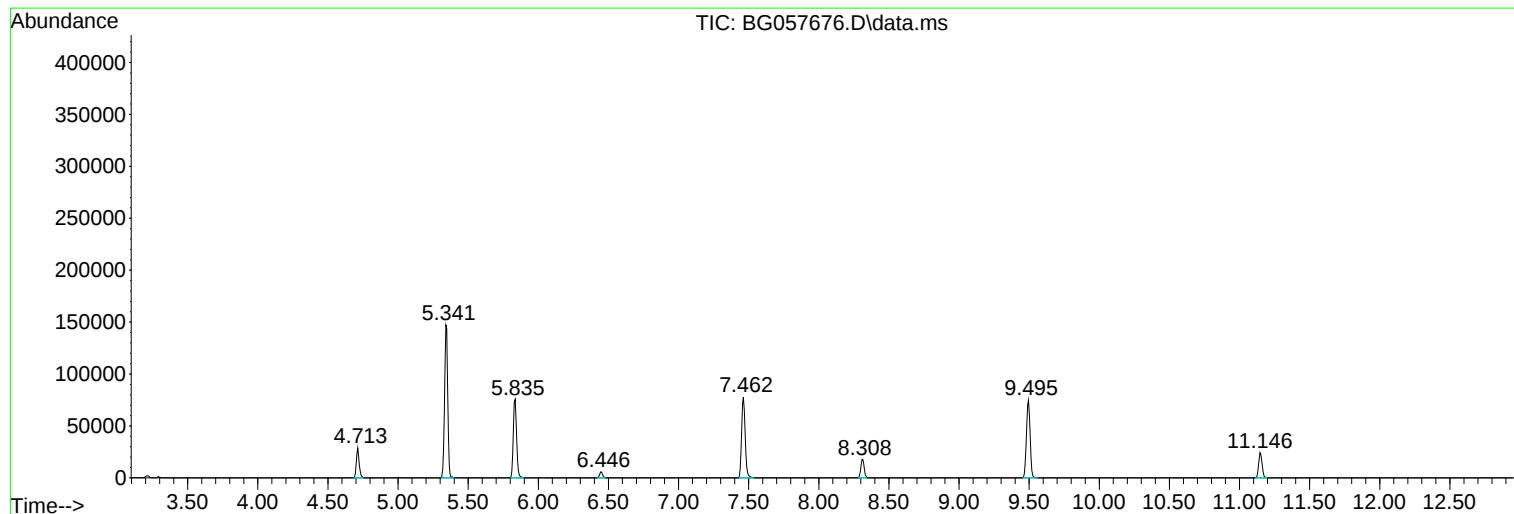
Sum of corrected areas: 2027095

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060823\
Data File : BG057676.D
Acq On : 8 Jun 2023 18:40
Operator : CG/JU
Sample : PB153189BL
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB153189BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060823\
Data File : BG057676.D
Acq On : 8 Jun 2023 18:40
Operator : CG/JU
Sample : PB153189BL
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB153189BL

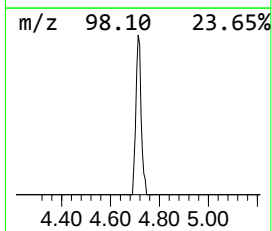
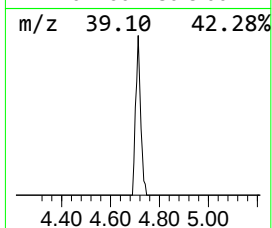
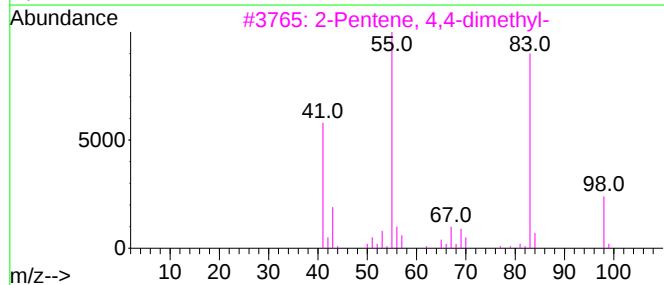
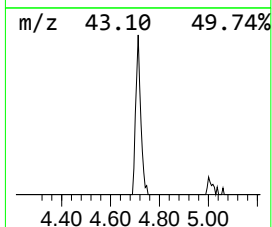
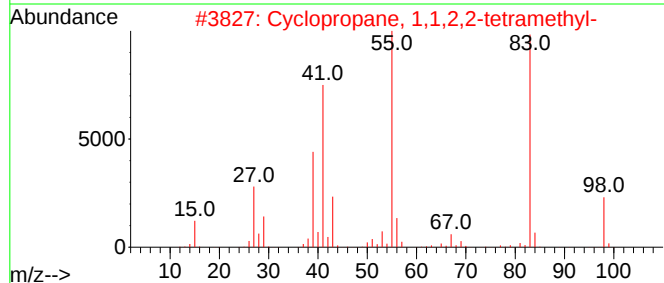
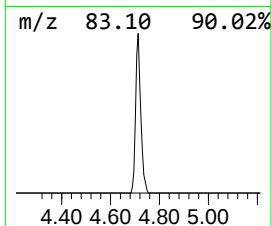
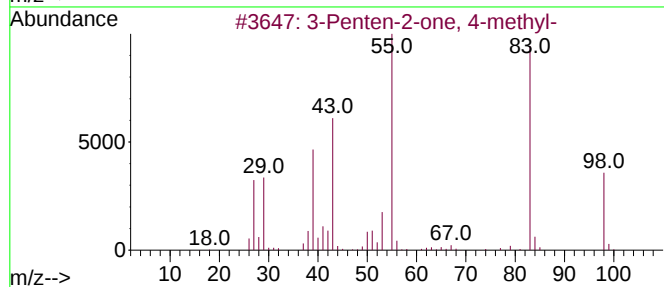
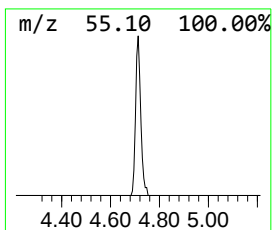
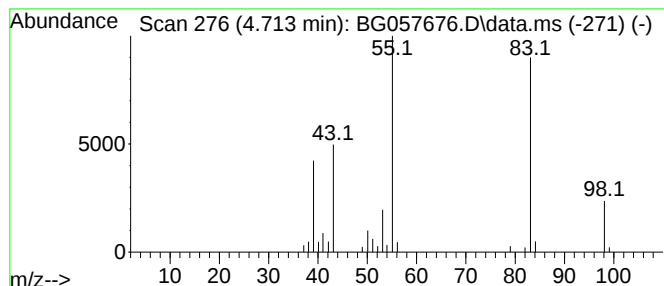
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.713	27.18 ng	40715	1,4-Dichlorobenzene-d4	8.314

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	86
2		Cyclopropane, 1,1,2,2-tetramethyl-	98	C7H14	004127-47-3	80
3		2-Pentene, 4,4-dimethyl-	98	C7H14	026232-98-4	64
4		1-Butene, 2,3,3-trimethyl-	98	C7H14	000594-56-9	64
5		1,4-Pentadien-3-ol	84	C5H8O	000922-65-6	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060823\
Data File : BG057676.D
Acq On : 8 Jun 2023 18:40
Operator : CG/JU
Sample : PB153189BL
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB153189BL

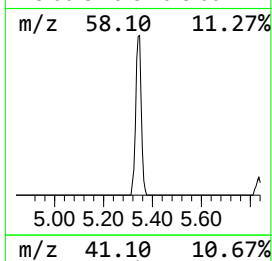
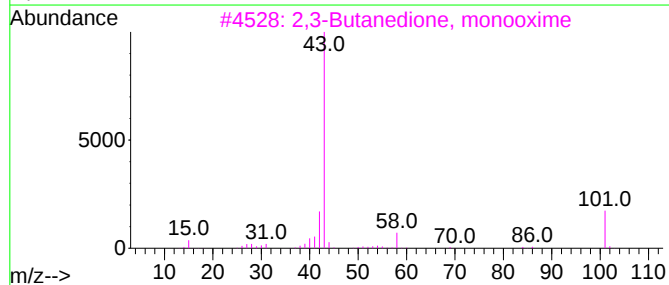
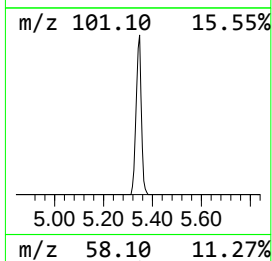
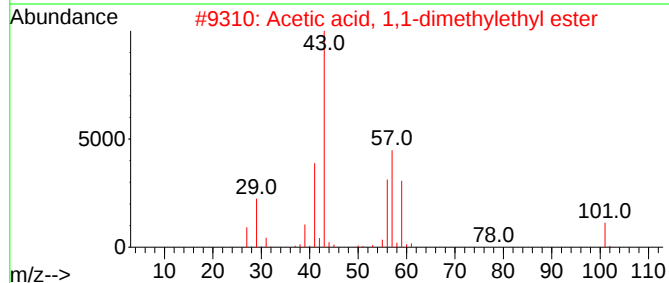
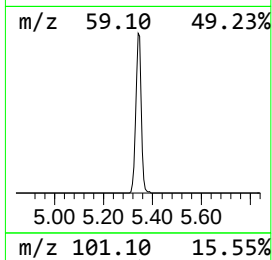
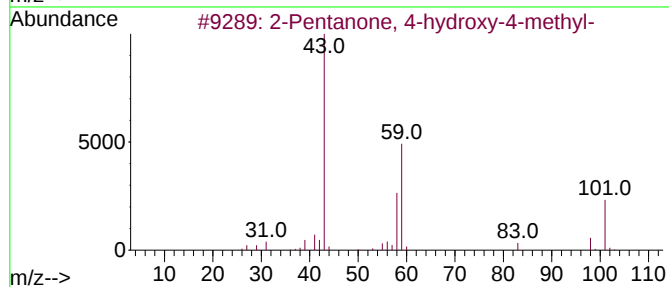
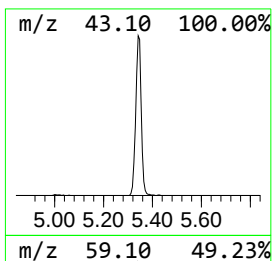
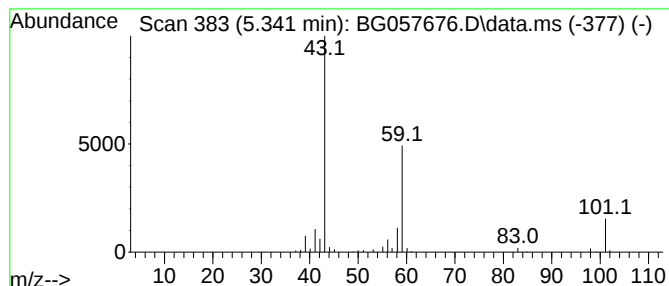
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.341	153.71 ng	230273	1,4-Dichlorobenzene-d4	8.314

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	28
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5			Butane	58	C4H10	000106-97-8	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060823\
Data File : BG057676.D
Acq On : 8 Jun 2023 18:40
Operator : CG/JU
Sample : PB153189BL
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB153189BL

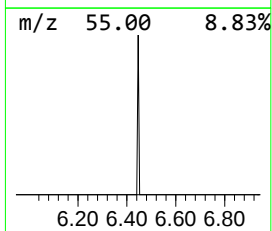
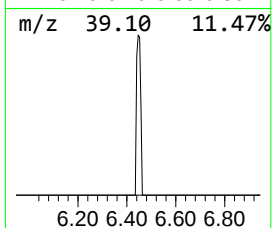
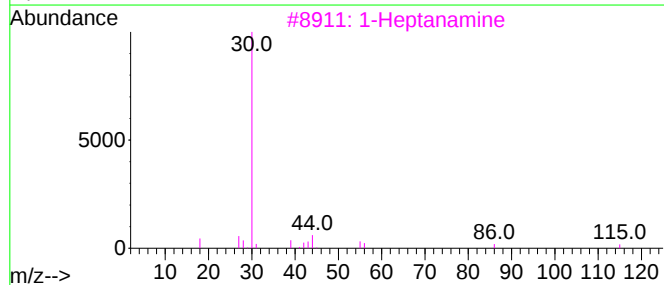
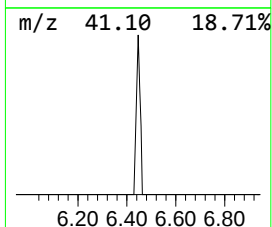
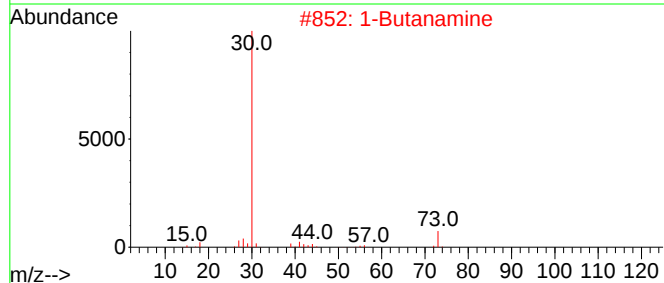
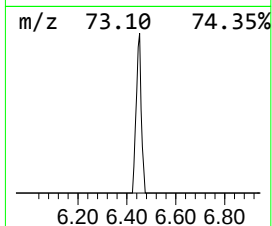
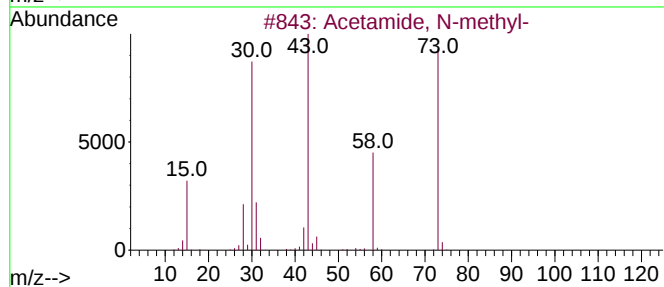
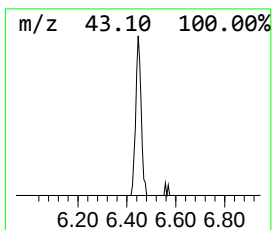
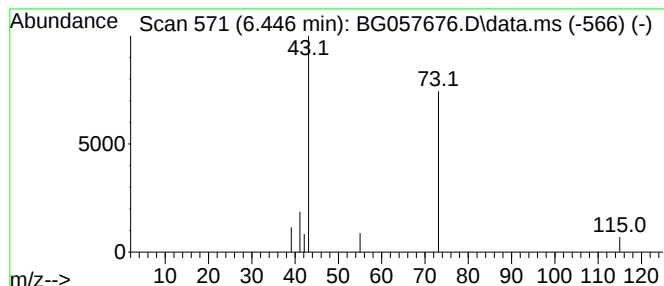
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.446 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.446	5.73 ng	8577	1,4-Dichlorobenzene-d4	8.314

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetamide, N-methyl-	73	C3H7NO	000079-16-3	5
2			1-Butanamine	73	C4H11N	000109-73-9	4
3			1-Heptanamine	115	C7H17N	000111-68-2	4
4			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	4
5			Guanidine, methyl-	73	C2H7N3	000471-29-4	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060823\
Data File : BG057676.D
Acq On : 8 Jun 2023 18:40
Operator : CG/JU
Sample : PB153189BL
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB153189BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one,...	4.713	27.2	ng	40715	1	8.314	29963	20.0
2-Pentanone, 4-...	5.341	153.7	ng	230273	1	8.314	29963	20.0
unknown6.446	6.446	5.7	ng	8577	1	8.314	29963	20.0