

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122023\
 Data File : BG060117.D
 Acq On : 21 Dec 2023 3:17
 Operator : MA/JU
 Sample : 05791-03
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 597-P-2

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-BG121323.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060117.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.138	3	8	19	rVB2	89627	182798	1.55%	0.614%
2	3.784	92	118	121	rBV	2408170	11815639	100.00%	39.670%
3	5.535	408	416	425	rBV	681258	1163118	9.84%	3.905%
4	7.121	676	686	696	rBV	656969	1164557	9.86%	3.910%
5	7.950	821	827	835	rBV	199176	336605	2.85%	1.130%
6	9.113	1017	1025	1034	rBV	426300	754209	6.38%	2.532%
7	10.752	1295	1304	1313	rBV	237634	439363	3.72%	1.475%
8	13.208	1716	1722	1732	rBV	1451637	2253213	19.07%	7.565%
9	14.589	1949	1957	1962	rBV	447480	691554	5.85%	2.322%
10	14.794	1984	1992	2000	rVB5	99562	234918	1.99%	0.789%
11	16.075	2202	2210	2221	rBV	1338257	2194564	18.57%	7.368%
12	17.339	2415	2425	2431	rBV	668509	1042258	8.82%	3.499%
13	19.395	2770	2775	2779	rBV	122194	153159	1.30%	0.514%
14	19.959	2865	2871	2881	rVB	3644478	4668146	39.51%	15.673%
15	21.610	3145	3152	3157	rBV	898892	1576309	13.34%	5.292%
16	24.800	3688	3695	3703	rBV	418327	1114421	9.43%	3.742%

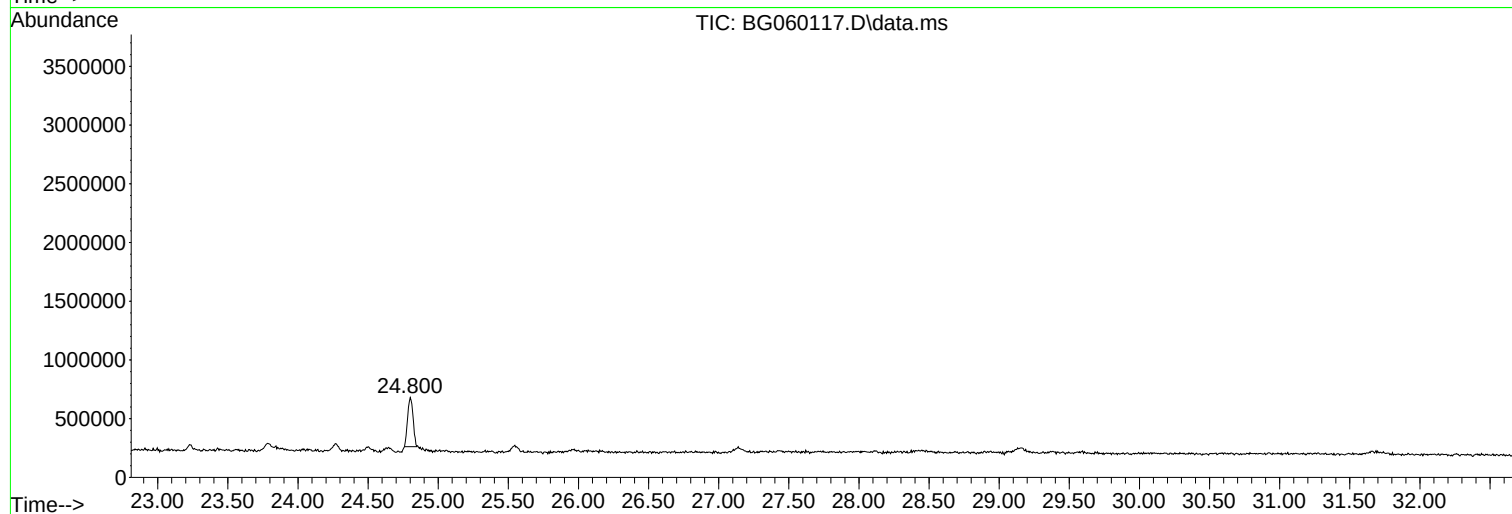
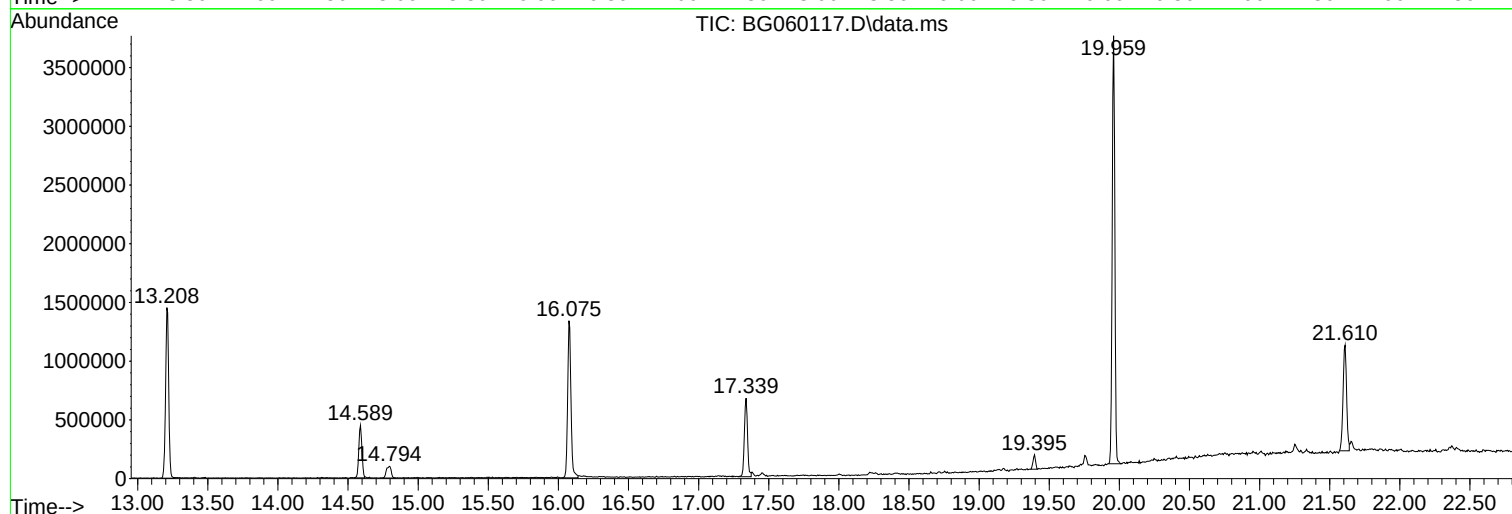
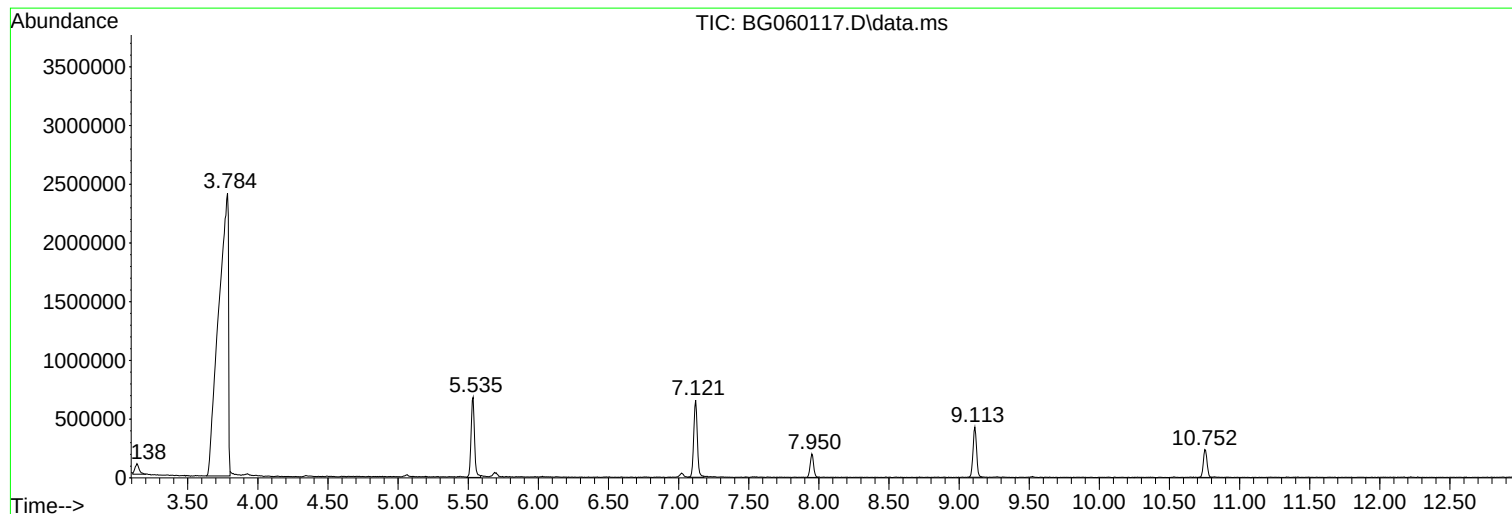
Sum of corrected areas: 29784831

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122023\
Data File : BG060117.D
Acq On : 21 Dec 2023 3:17
Operator : MA/JU
Sample : 05791-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
597-P-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.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\BG122023\
Data File : BG060117.D
Acq On : 21 Dec 2023 3:17
Operator : MA/JU
Sample : 05791-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
597-P-2

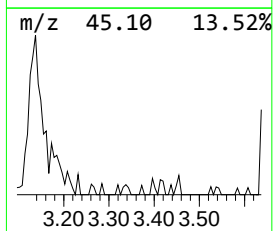
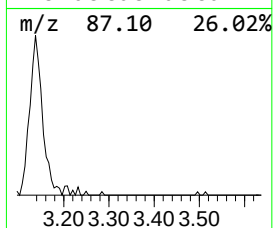
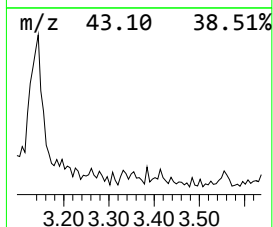
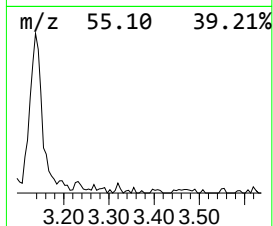
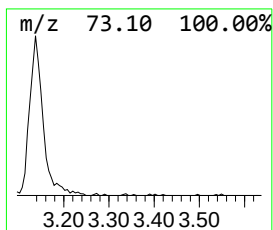
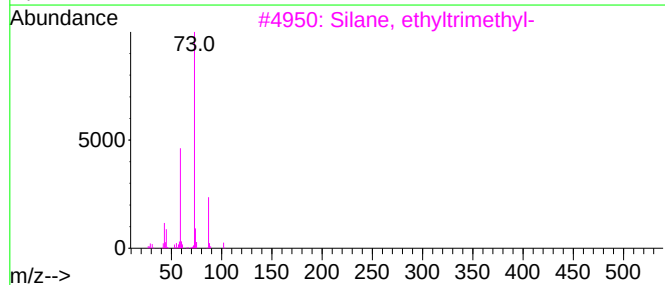
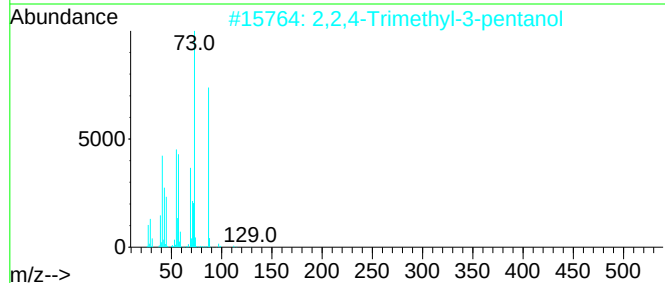
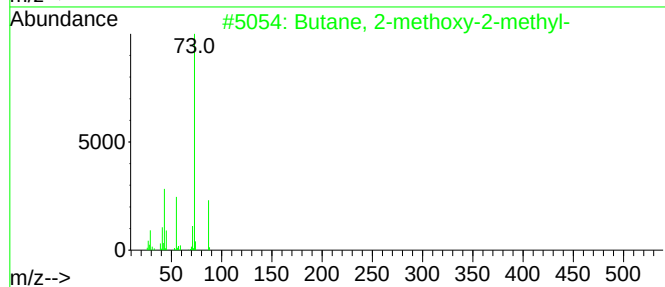
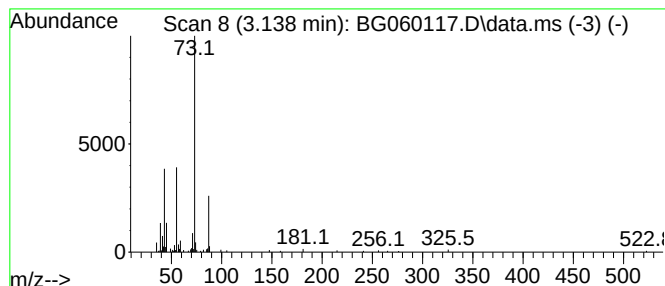
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.138	10.86 ng	182798	1,4-Dichlorobenzene-d4	7.950

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	50
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	36
3			Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	33
4			3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	28
5			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	17



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122023\
Data File : BG060117.D
Acq On : 21 Dec 2023 3:17
Operator : MA/JU
Sample : 05791-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
597-P-2

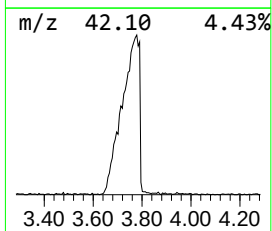
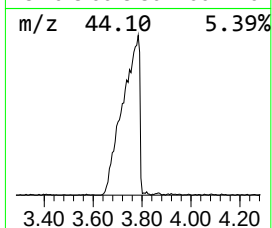
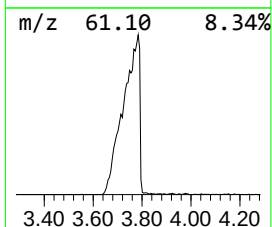
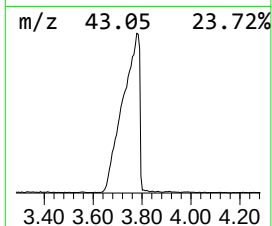
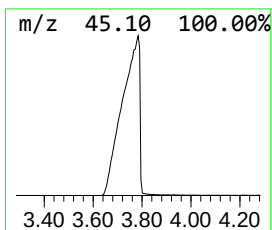
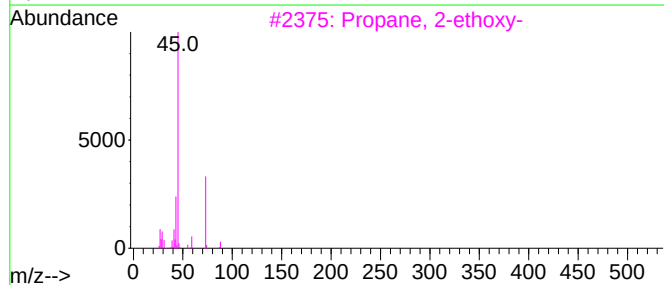
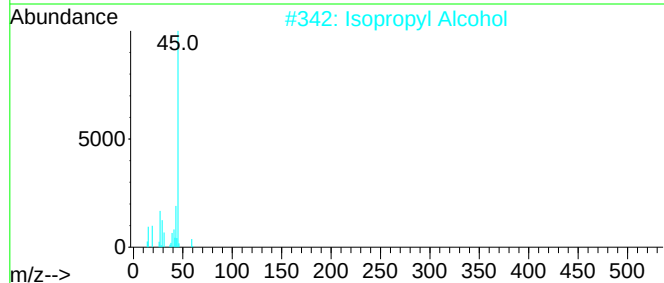
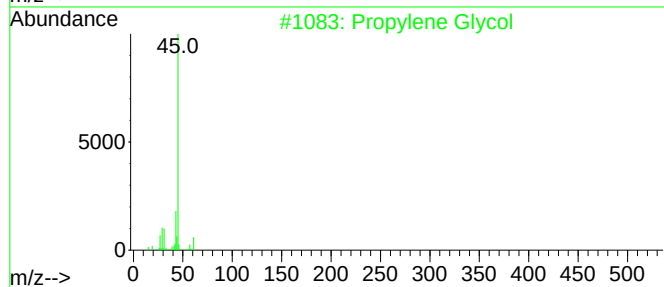
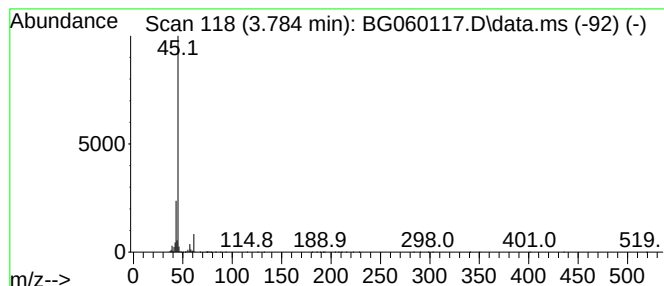
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Propylene Glycol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.784	702.05 ng	11815600	1,4-Dichlorobenzene-d4	7.950

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	83
2			Isopropyl Alcohol	60	C3H8O	000067-63-0	56
3			Propane, 2-ethoxy-	88	C5H12O	000625-54-7	39
4			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9
5			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122023\
Data File : BG060117.D
Acq On : 21 Dec 2023 3:17
Operator : MA/JU
Sample : 05791-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
597-P-2

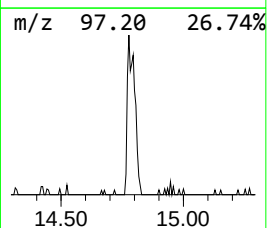
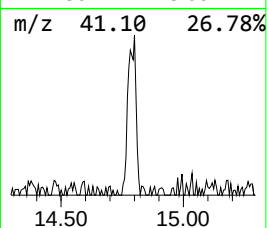
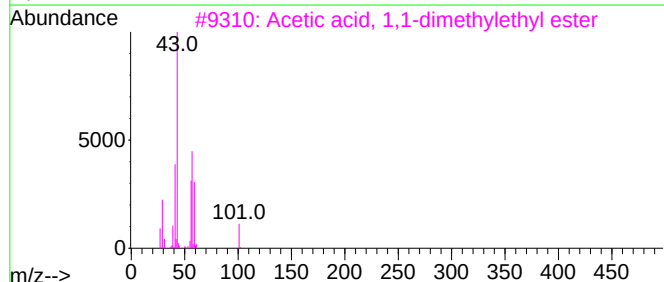
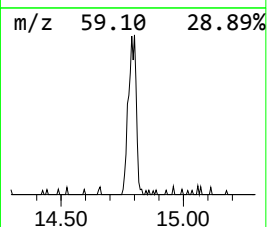
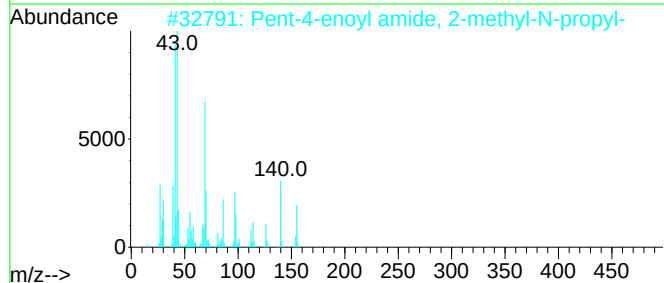
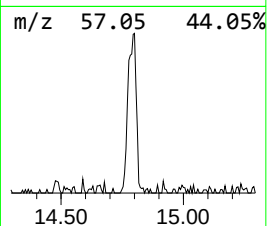
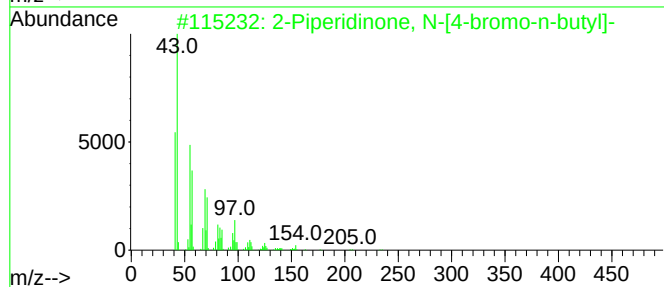
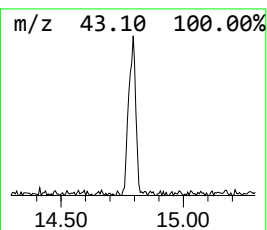
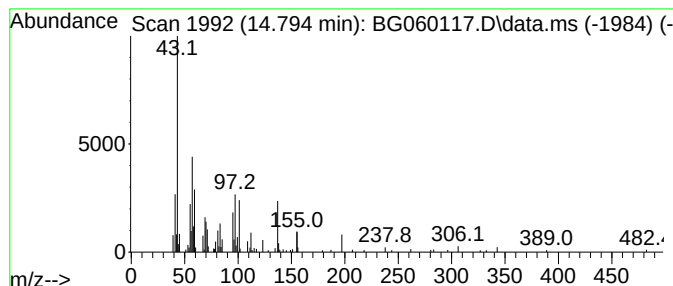
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown14.794 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.794	6.79 ng	234918	Acenaphthene-d10	14.589

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Piperidinone, N-[4-bromo-n-but...	233	C9H16BrNO	195194-80-0	12
2			Pent-4-enoyl amide, 2-methyl-N-p...	155	C9H17NO	1000420-35-2	12
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	12
4			Methyl 6-oxoheptanoate	158	C8H14O3	002046-21-1	12
5			4-Pyridinol, acetate (ester)	137	C7H7NO2	014210-20-9	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122023\
Data File : BG060117.D
Acq On : 21 Dec 2023 3:17
Operator : MA/JU
Sample : 05791-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
597-P-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.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
Butane, 2-metho...	3.138	10.9	ng	182798	1	7.950	336605	20.0
Propylene Glycol	3.784	702.0	ng	11815600	1	7.950	336605	20.0
unknown14.794	14.794	6.8	ng	234918	3	14.589	691554	20.0