

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
 Data File : BF139114.D
 Acq On : 22 Aug 2024 10:54
 Operator : RC/JU
 Sample : PB162782BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB162782BL

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_F\Methods\8270-BF082024.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139114.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.287	19	33	42	rVB	62737	116620	2.69%	0.501%
2	5.140	509	518	527	rBV	117388	194143	4.48%	0.834%
3	5.522	576	583	589	rBV	2127149	3034066	70.03%	13.028%
4	6.522	745	753	758	rBV	2061379	3111934	71.82%	13.362%
5	6.898	812	817	822	rVB	438014	552997	12.76%	2.375%
6	7.457	905	912	917	rBV	1446696	1992808	45.99%	8.557%
7	8.175	1028	1034	1039	rBV	552437	714989	16.50%	3.070%
8	9.257	1210	1218	1223	rBV	2606961	3620505	83.56%	15.546%
9	9.934	1327	1333	1338	rBV	666182	837756	19.34%	3.597%
10	10.722	1460	1467	1472	rBV	1812064	2386923	55.09%	10.249%
11	11.416	1580	1585	1590	rBV	721930	902954	20.84%	3.877%
12	13.010	1850	1856	1861	rBV	3301316	4332689	100.00%	18.604%
13	14.057	2028	2034	2039	rVB	635402	802815	18.53%	3.447%
14	15.533	2279	2285	2291	rBV	420013	624981	14.42%	2.684%
15	17.198	2558	2568	2587	rVB5	12603	62789	1.45%	0.270%

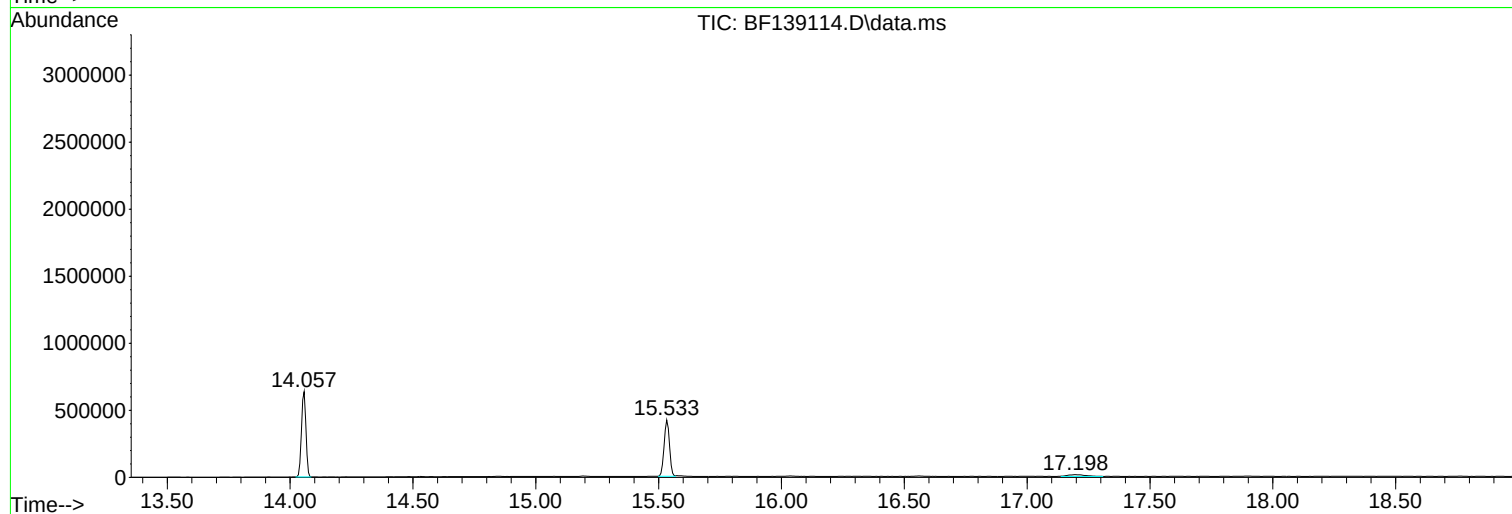
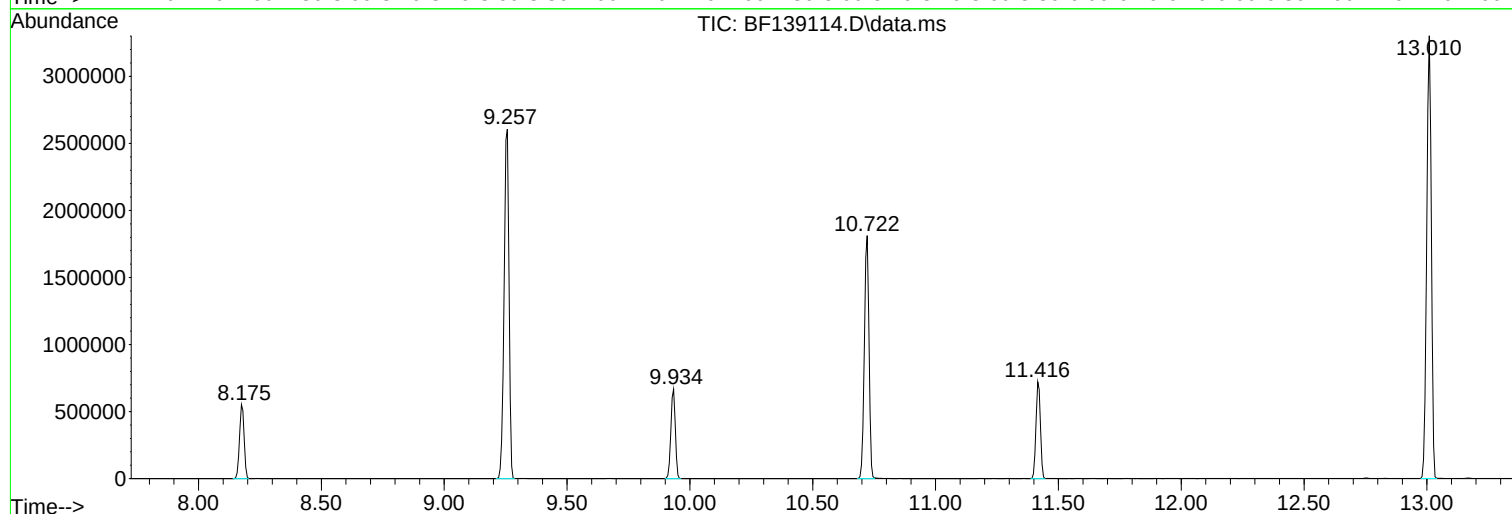
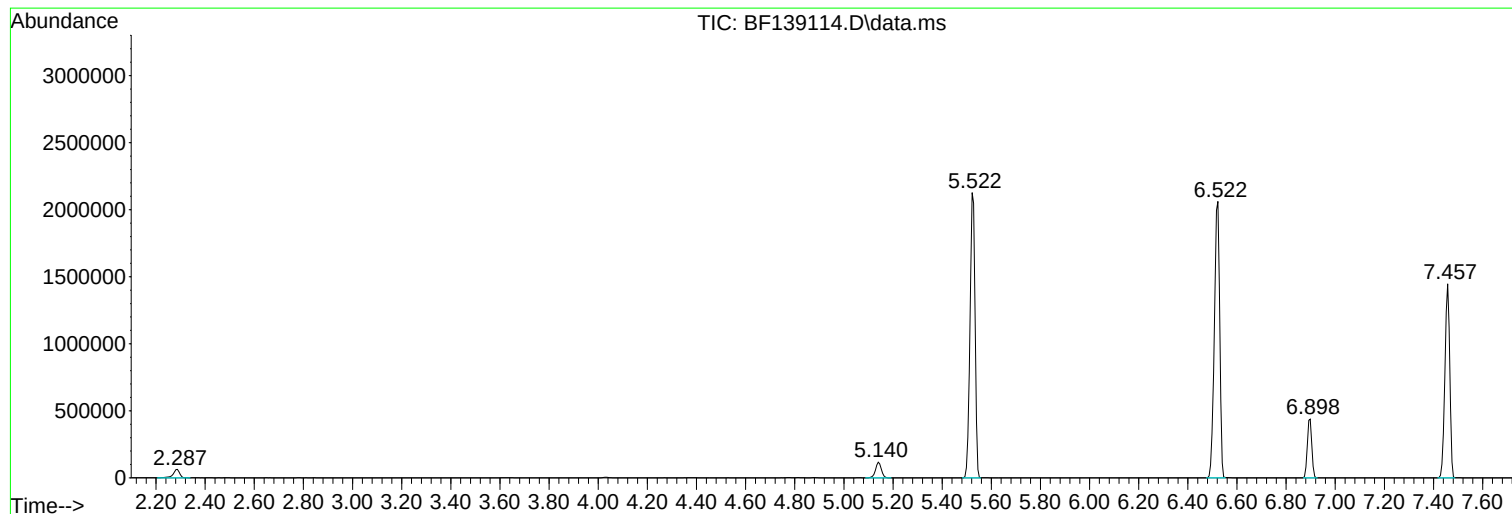
Sum of corrected areas: 23288969

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139114.D
Acq On : 22 Aug 2024 10:54
Operator : RC/JU
Sample : PB162782BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB162782BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.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_F\Data\BF082224\
Data File : BF139114.D
Acq On : 22 Aug 2024 10:54
Operator : RC/JU
Sample : PB162782BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB162782BL

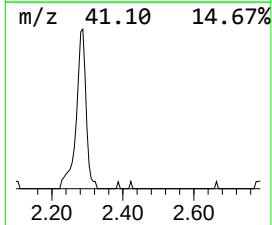
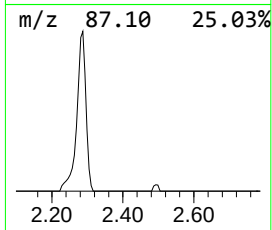
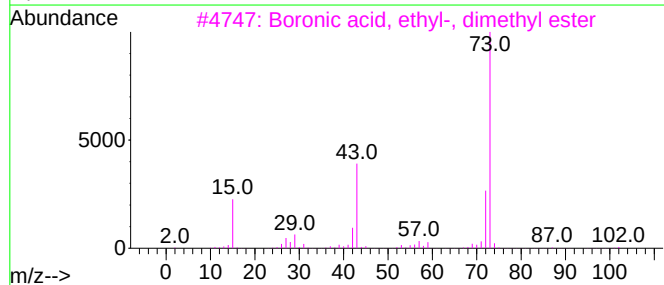
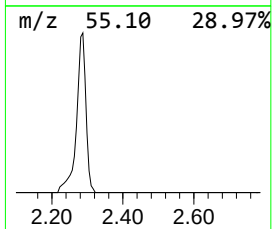
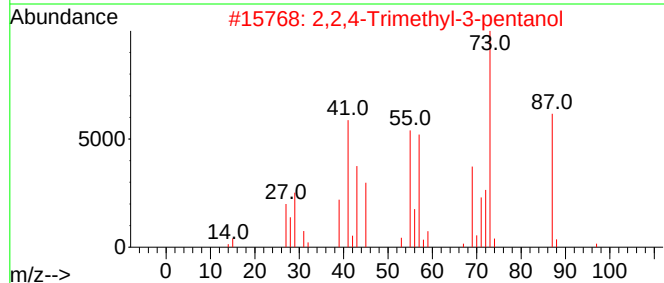
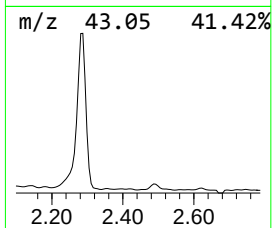
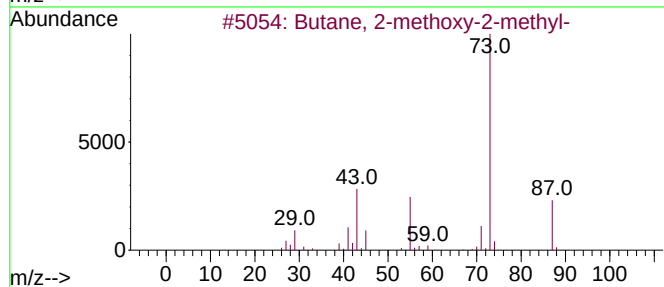
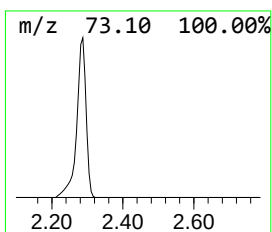
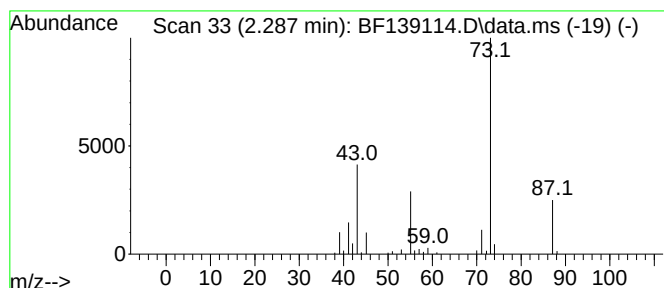
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.287	4.22 ng	116620	1,4-Dichlorobenzene-d4	6.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	17
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139114.D
Acq On : 22 Aug 2024 10:54
Operator : RC/JU
Sample : PB162782BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB162782BL

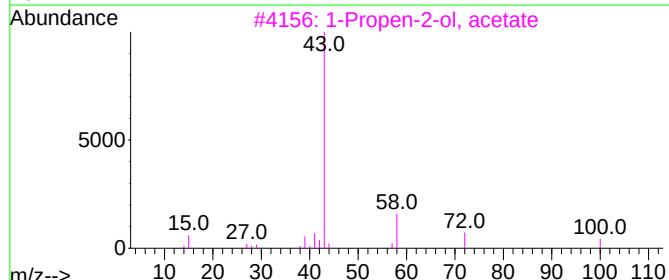
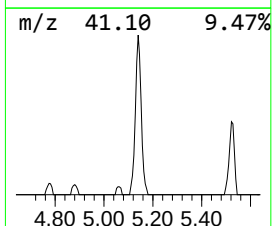
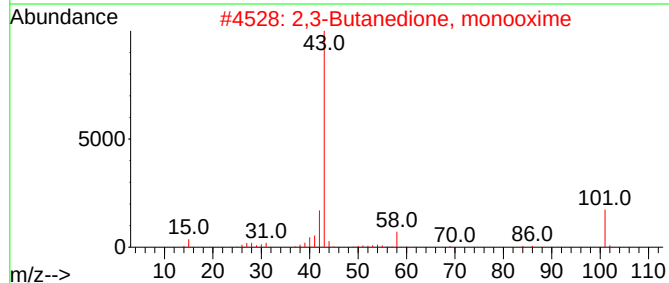
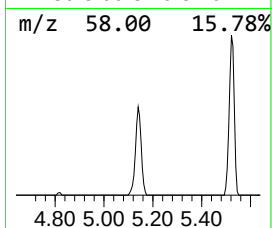
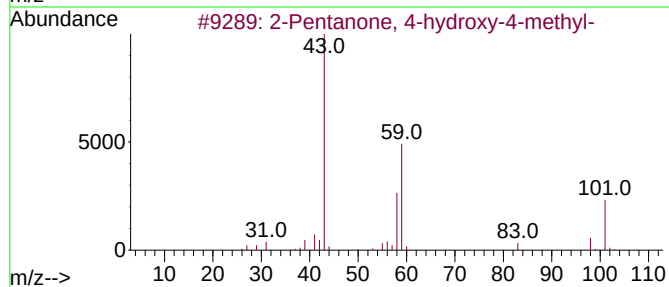
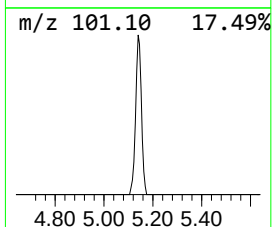
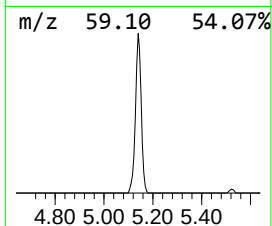
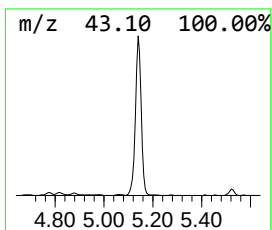
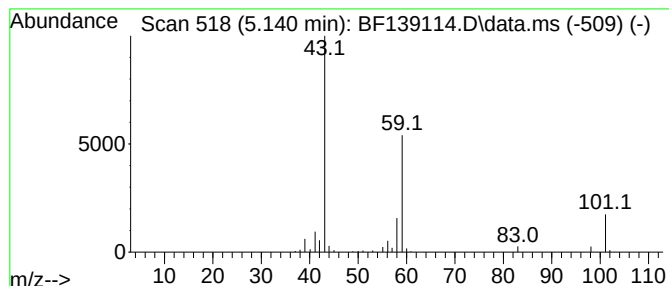
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.140	7.02 ng	194143	1,4-Dichlorobenzene-d4	6.898

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4		Butane	58	C4H10	000106-97-8	9
5		Acetone	58	C3H6O	000067-64-1	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139114.D
Acq On : 22 Aug 2024 10:54
Operator : RC/JU
Sample : PB162782BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

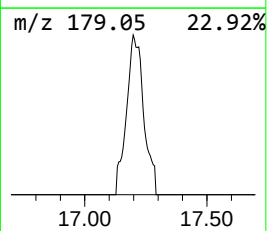
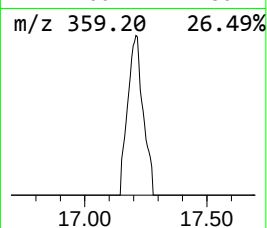
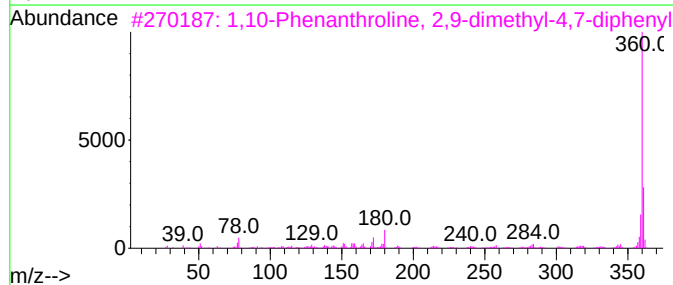
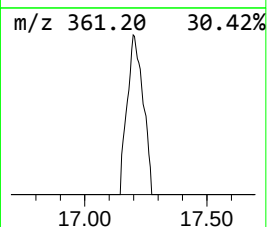
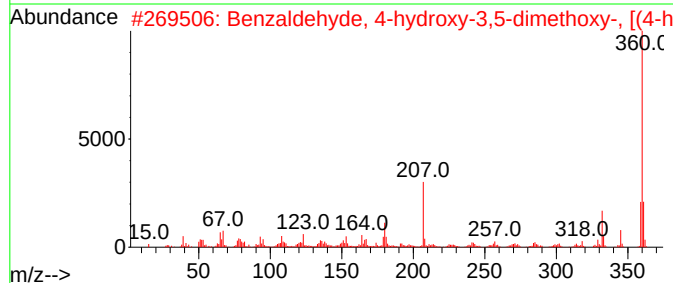
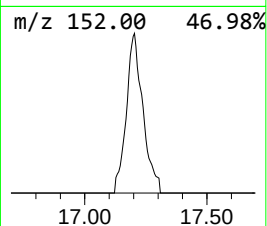
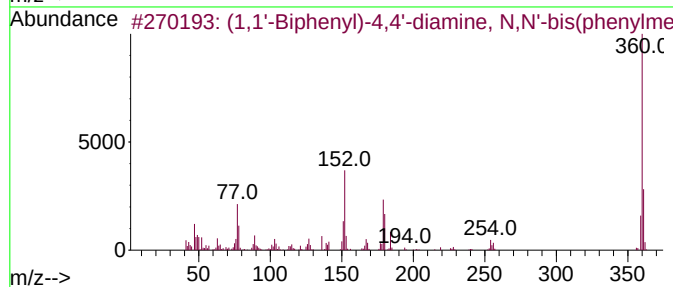
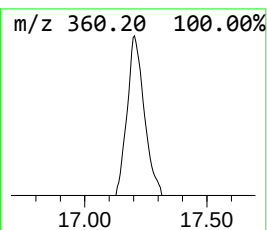
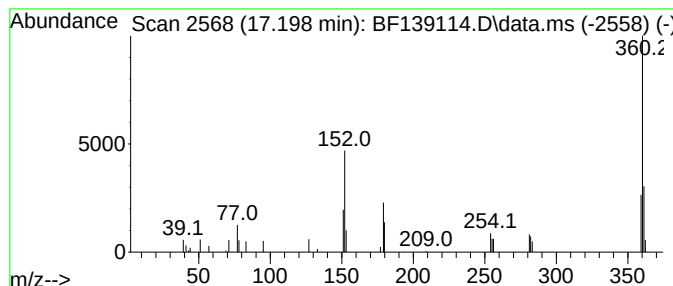
Instrument :
BNA_F
ClientSampleId :
PB162782BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 (1,1'-Biphenyl)-4,4'-diamin... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.198	2.01 ng	62789	Perylene-d12	15.533	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1,1'-Biphenyl)-4,4'-diamine, N,N'-bis(4-chlorophenyl)	360	C26H20N2	006311-48-4	90
2	Benzaldehyde, 4-hydroxy-3,5-dimethoxy	360	C18H20N2O6	014414-32-5	46
3	1,10-Phenanthroline, 2,9-dimethyl	360	C26H20N2	004733-39-5	43
4	Pentacyclo[18.4.1.1(2,7).1(8,13).0(9,16)]octa-2,4,6,8-tetraene	360	C28H24	101077-60-5	43
5	1,3,2-Dioxaborolane, bis(spiro[4.5]undec-8-en-2-ylidene)	360	C20H13B06	1000150-23-7	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139114.D
Acq On : 22 Aug 2024 10:54
Operator : RC/JU
Sample : PB162782BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB162782BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.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...	2.287	4.2	ng	116620	1	6.898	552997	20.0
2-Pentanone, 4-...	5.140	7.0	ng	194143	1	6.898	552997	20.0
(1,1'-Biphenyl)...	17.198	2.0	ng	62789	6	15.533	624981	20.0