

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050321\
 Data File : BF123785.D
 Acq On : 3 May 2021 18:10
 Operator : JU/CG
 Sample : PB136120BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB136120BL

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-BF042721.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123785.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.116	3	5	11	rVB	432074	475623	6.05%	0.866%
2	2.222	17	23	31	rVB	369651	452687	5.76%	0.824%
3	5.034	492	501	508	rBV	300261	423771	5.39%	0.772%
4	5.439	565	570	573	rBV	8322145	7815803	99.44%	14.231%
5	6.445	736	741	744	rBV	7392741	7859702	100.00%	14.310%
6	6.804	799	802	806	rBV	2005599	1549238	19.71%	2.821%
7	7.369	892	898	901	rBV	5004327	5196982	66.12%	9.462%
8	8.092	1016	1021	1024	rBV	2238481	1986475	25.27%	3.617%
9	9.169	1198	1204	1207	rBV	8393223	7701533	97.99%	14.023%
10	9.845	1313	1319	1323	rBV	2410947	2040215	25.96%	3.715%
11	10.633	1447	1453	1457	rBV	5112203	5166388	65.73%	9.407%
12	11.333	1567	1572	1575	rBV	2350453	2078674	26.45%	3.785%
13	11.863	1657	1662	1669	rBV6	47100	95252	1.21%	0.173%
14	12.927	1836	1843	1846	rBV	7565290	7825867	99.57%	14.249%
15	13.974	2014	2021	2024	rBV	2229121	1998955	25.43%	3.640%
16	15.427	2262	2268	2273	rBV	1465959	1880472	23.93%	3.424%
17	15.539	2278	2287	2298	rVB5	117436	374990	4.77%	0.683%

Sum of corrected areas: 54922627

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050321\
Data File : BF123785.D
Acq On : 3 May 2021 18:10
Operator : JU/CG
Sample : PB136120BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB136120BL

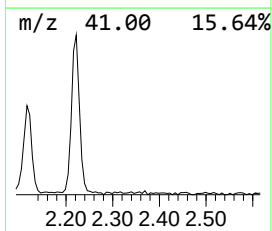
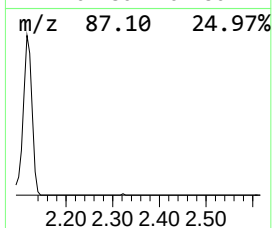
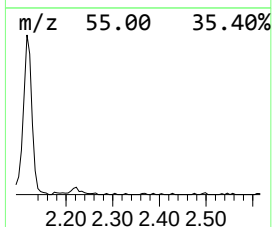
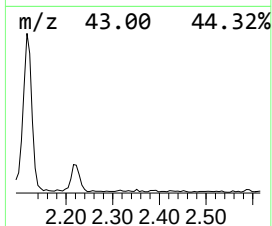
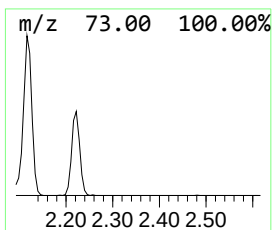
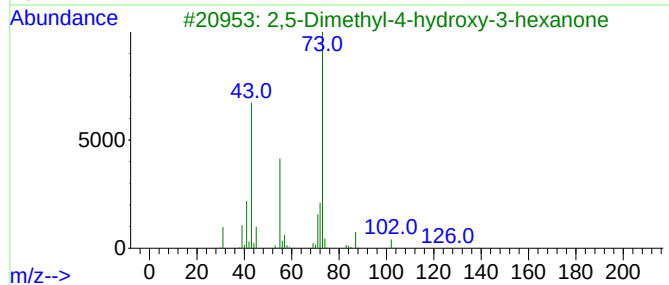
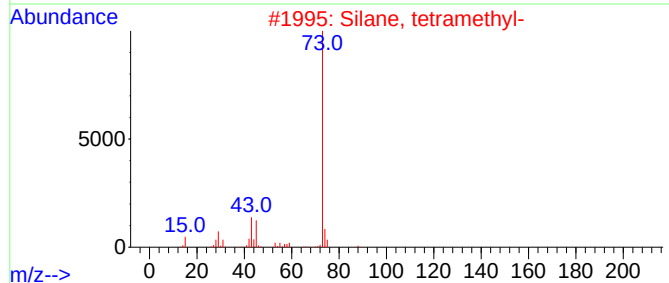
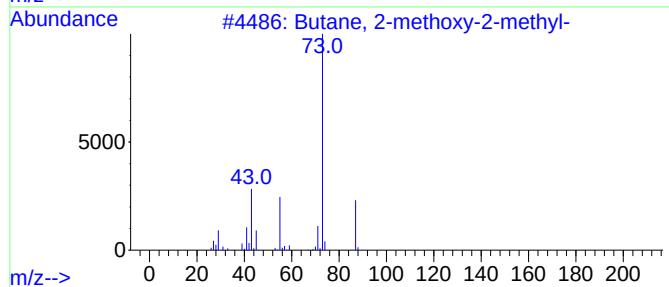
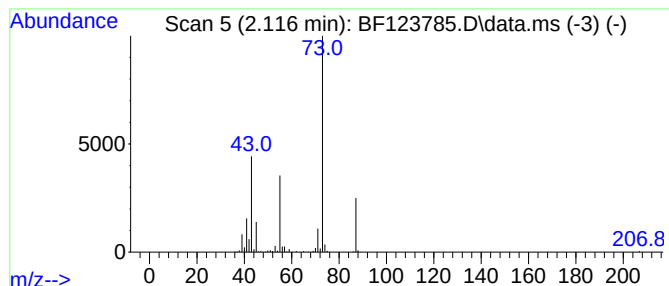
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.116	6.14 ng	475623	1,4-Dichlorobenzene-d4	6.804

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	56
2			Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
3			2,5-Dimethyl-4-hydroxy-3-hexanone	144	C8H16O2	000815-77-0	25
4			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	17



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050321\
Data File : BF123785.D
Acq On : 3 May 2021 18:10
Operator : JU/CG
Sample : PB136120BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB136120BL

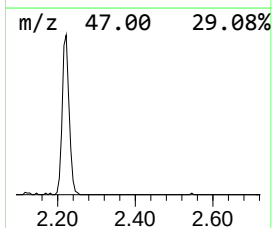
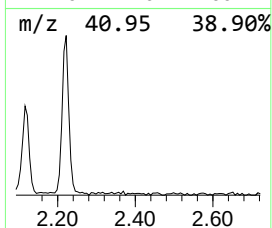
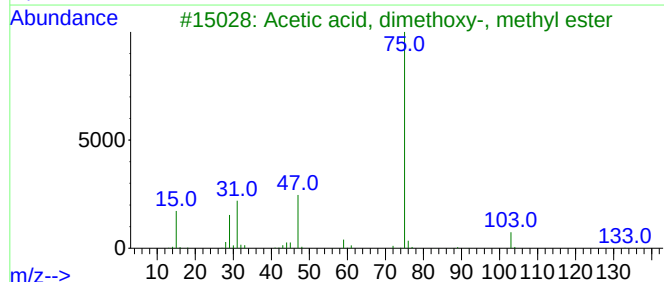
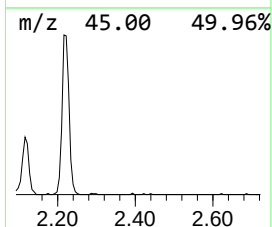
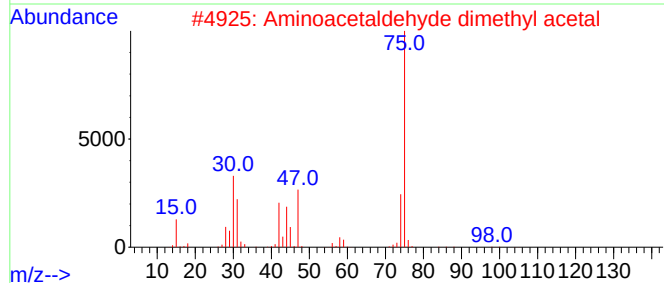
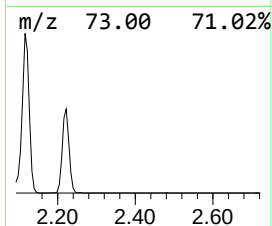
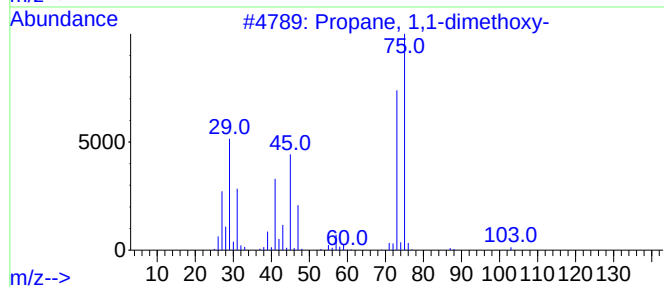
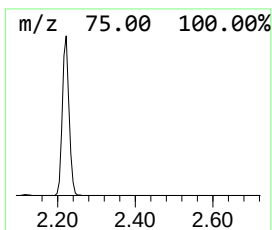
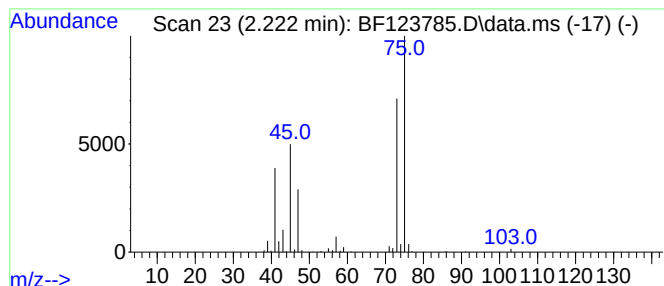
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.222	5.84 ng	452687	1,4-Dichlorobenzene-d4	6.804

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	78
2			Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	36
3			Acetic acid, dimethoxy-, methyl ...	134	C5H10O4	000089-91-8	33
4			Methane, trimethoxy-	106	C4H10O3	000149-73-5	33
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050321\
Data File : BF123785.D
Acq On : 3 May 2021 18:10
Operator : JU/CG
Sample : PB136120BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB136120BL

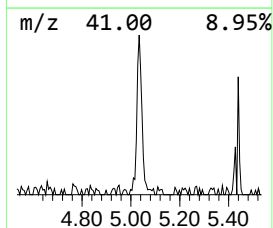
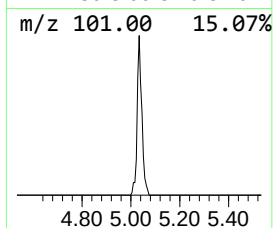
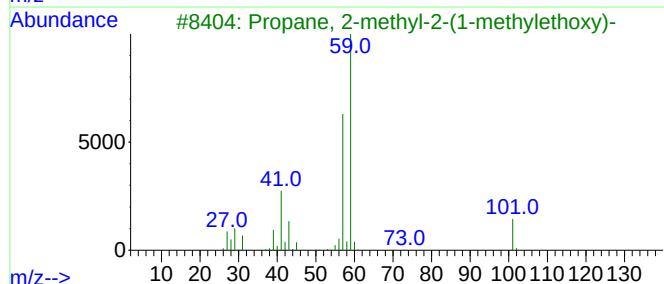
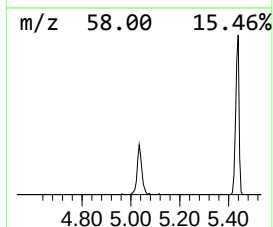
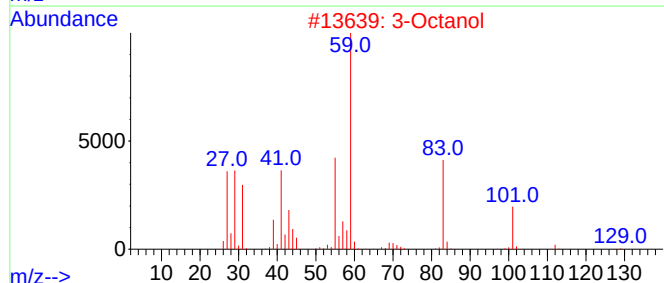
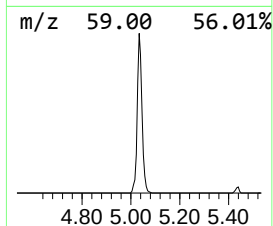
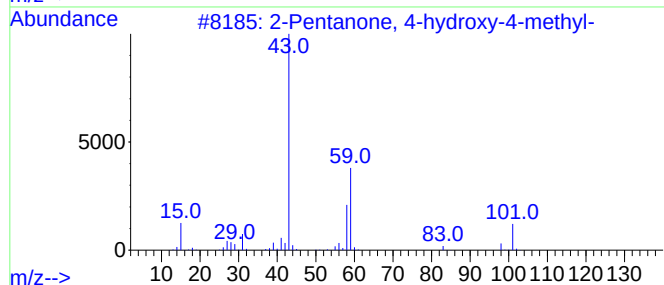
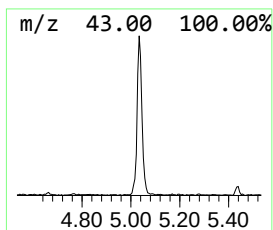
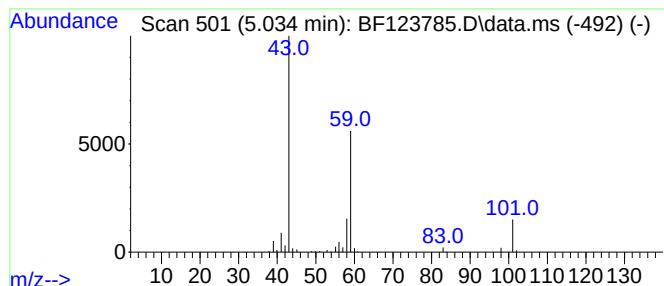
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.034	5.47 ng	423771	1,4-Dichlorobenzene-d4	6.804

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			3-Octanol	130	C8H18O	000589-98-0	33
3			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050321\
Data File : BF123785.D
Acq On : 3 May 2021 18:10
Operator : JU/CG
Sample : PB136120BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB136120BL

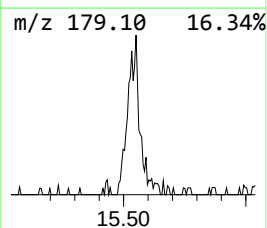
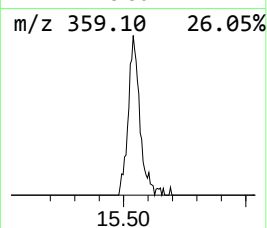
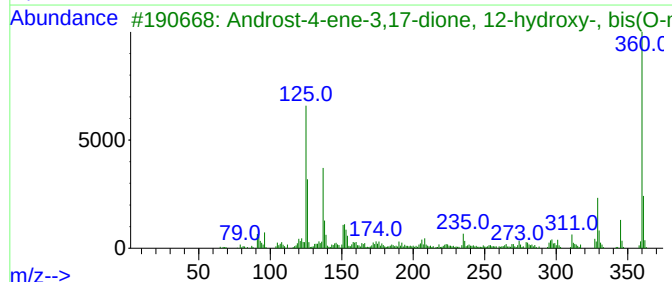
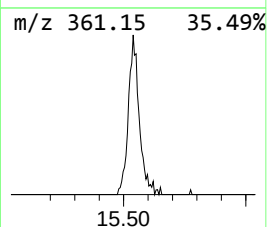
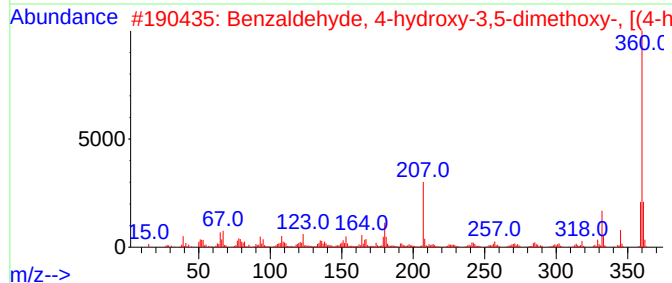
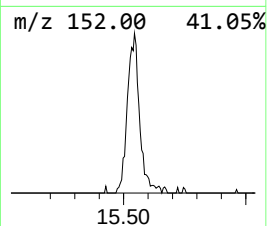
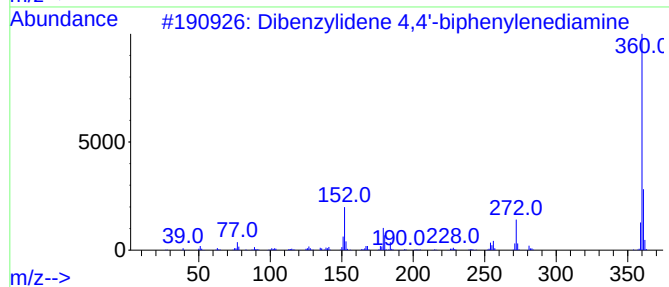
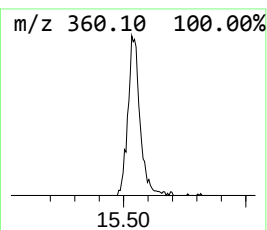
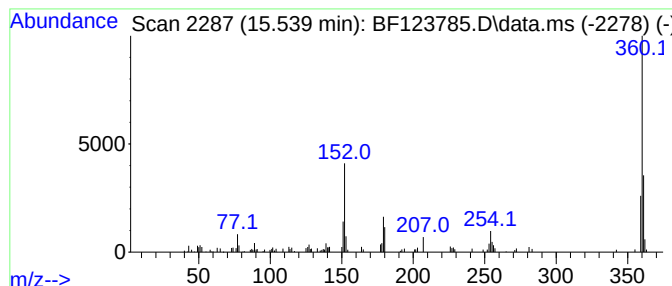
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Dibenzylidene 4,4'-biphenyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.539	3.99 ng	374990	Perylene-d12	15.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dibenzylidene 4,4'-biphenylenedi...	360	C26H20N2	006311-48-4	90
2			Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	50
3			Androst-4-ene-3,17-dione, 12-hyd...	360	C21H32N2O3	069688-31-9	47
4			1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	47
5			N,N'-di-2-Naphthyl-p-phenylenedi...	360	C26H20N2	000093-46-9	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050321\
Data File : BF123785.D
Acq On : 3 May 2021 18:10
Operator : JU/CG
Sample : PB136120BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB136120BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.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
Butane, 2-metho...	2.116	6.1	ng	475623	1	6.804	1549240	20.0
Propane, 1,1-di...	2.222	5.8	ng	452687	1	6.804	1549240	20.0
2-Pentanone, 4-...	5.034	5.5	ng	423771	1	6.804	1549240	20.0
Dibenzylidene 4...	15.539	4.0	ng	374990	6	15.433	1880470	20.0