

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050521\
 Data File : BF123824.D
 Acq On : 5 May 2021 13:12
 Operator : JU/CG
 Sample : PB136166BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB136166BL

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: BF123824.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.204	16	20	28	rVB	252100	317257	3.74%	0.545%
2	5.022	495	499	508	rVB	413914	543447	6.41%	0.934%
3	5.428	563	568	571	rBV	8553497	8217046	96.97%	14.117%
4	6.439	734	740	743	rBV	7855953	8292666	97.86%	14.247%
5	6.792	797	800	804	rBV	2135927	1657567	19.56%	2.848%
6	7.363	891	897	899	rBV	4974503	5566343	65.69%	9.563%
7	8.081	1014	1019	1022	rBV	2450846	2168446	25.59%	3.725%
8	9.157	1196	1202	1205	rBV	8413926	8473950	100.00%	14.558%
9	9.833	1312	1317	1321	rBV	2646508	2309479	27.25%	3.968%
10	10.627	1446	1452	1455	rBV	6077496	5537264	65.34%	9.513%
11	11.321	1566	1570	1574	rBV	2726460	2358706	27.83%	4.052%
12	12.921	1836	1842	1845	rBV	8090446	8351971	98.56%	14.349%
13	13.839	1994	1998	2004	rVB	124311	136162	1.61%	0.234%
14	13.968	2016	2020	2024	rBV	2353348	1964788	23.19%	3.376%
15	15.427	2262	2268	2272	rBV	1450016	1739692	20.53%	2.989%
16	16.774	2484	2497	2510	rBV4	149048	572160	6.75%	0.983%

Sum of corrected areas: 58206944

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050521\
Data File : BF123824.D
Acq On : 5 May 2021 13:12
Operator : JU/CG
Sample : PB136166BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB136166BL

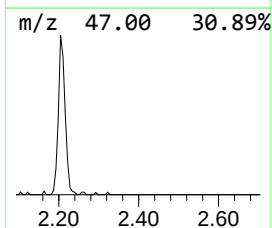
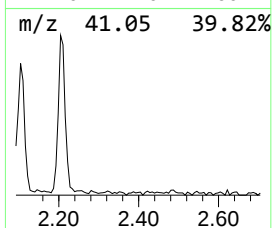
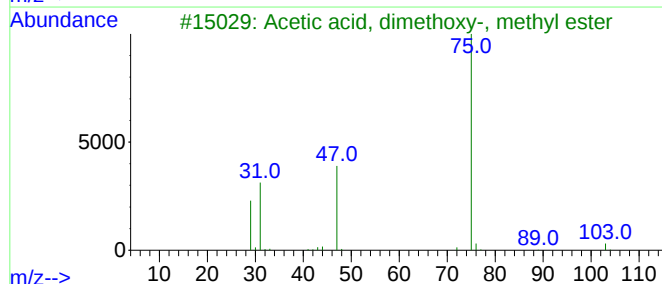
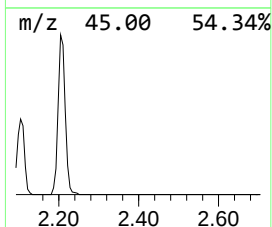
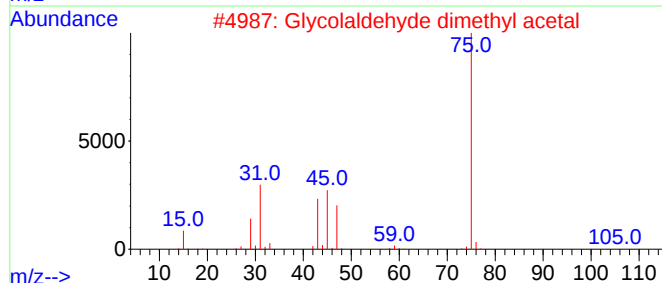
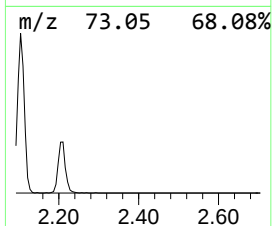
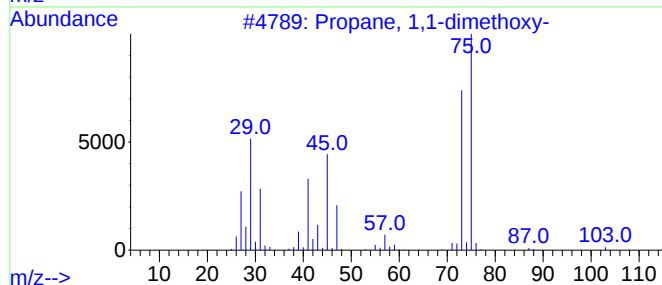
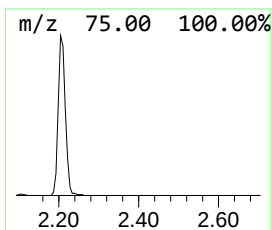
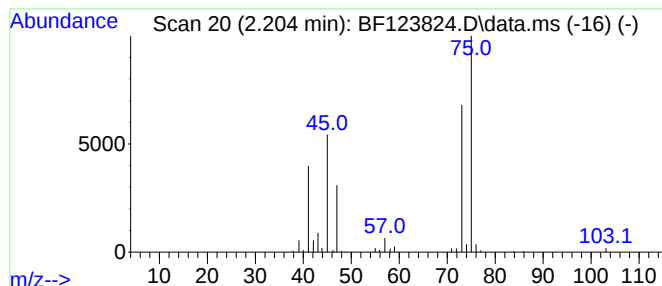
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.204	3.83 ng	317257	1,4-Dichlorobenzene-d4	6.792

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	78
2			Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	45
3			Acetic acid, dimethoxy-, methyl ...	134	C5H10O4	000089-91-8	40
4			Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	36
5			Methane, trimethoxy-	106	C4H10O3	000149-73-5	33



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050521\
Data File : BF123824.D
Acq On : 5 May 2021 13:12
Operator : JU/CG
Sample : PB136166BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB136166BL

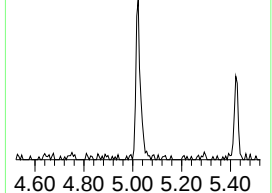
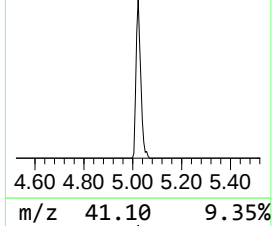
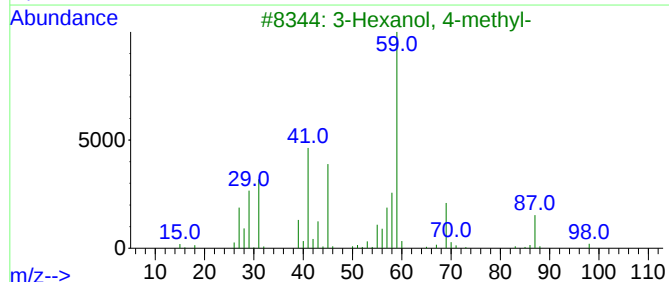
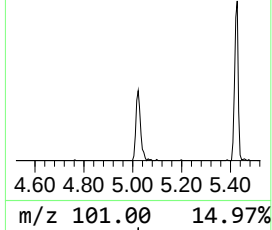
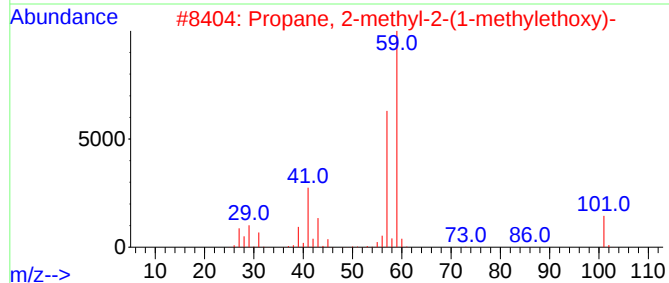
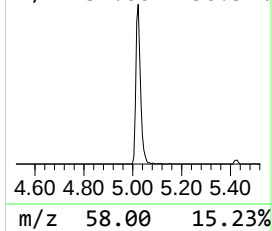
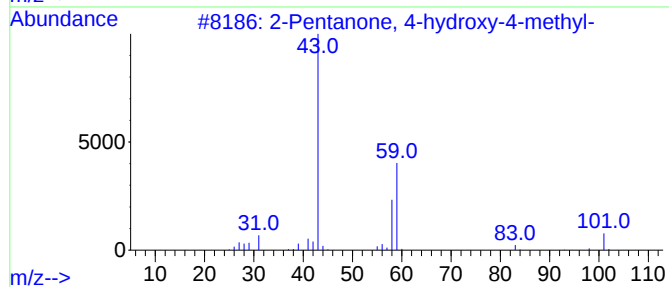
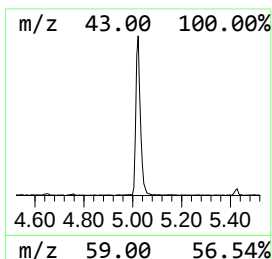
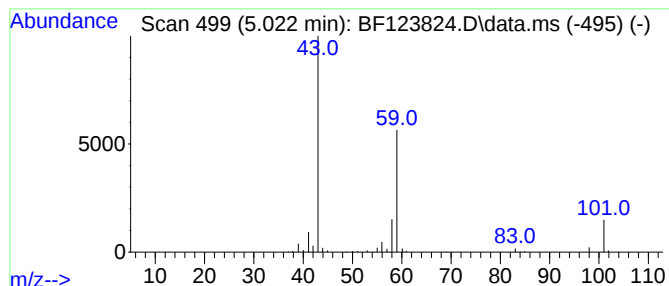
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.022	6.56 ng	543447	1,4-Dichlorobenzene-d4	6.792

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050521\
Data File : BF123824.D
Acq On : 5 May 2021 13:12
Operator : JU/CG
Sample : PB136166BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB136166BL

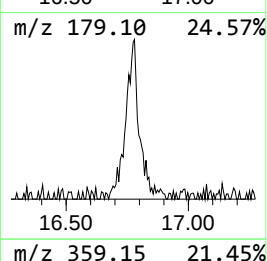
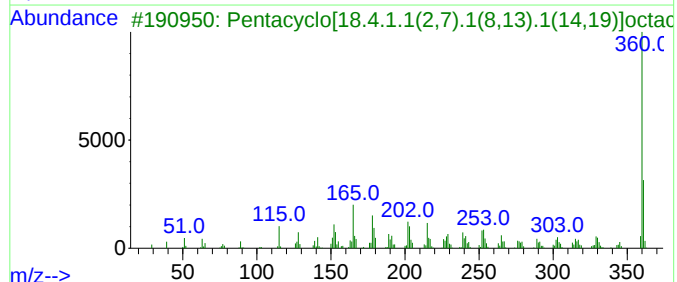
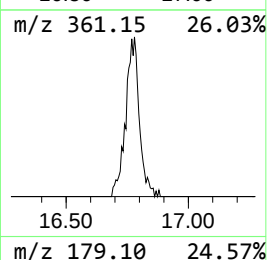
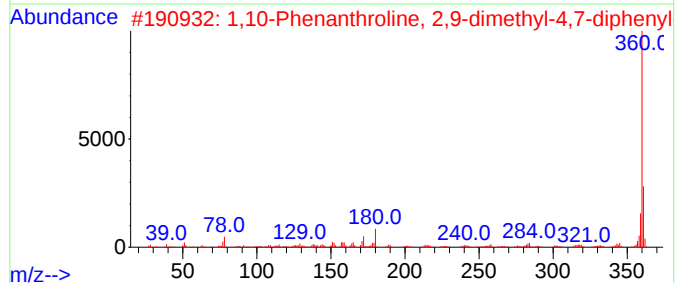
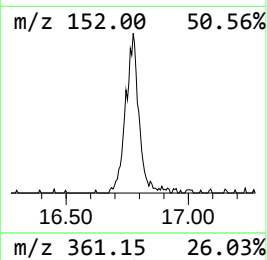
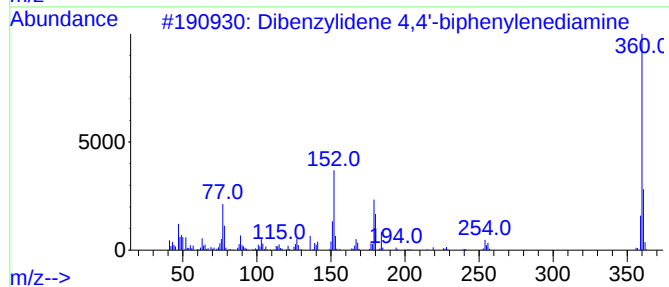
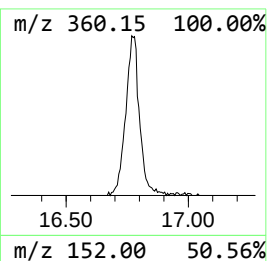
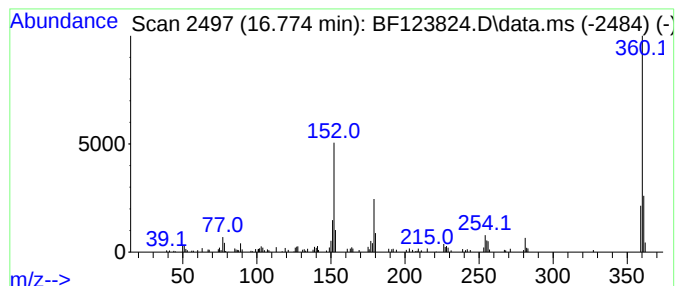
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Dibenzylidene 4,4'-biphenyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.774	6.58 ng	572160	Perylene-d12	15.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dibenzylidene 4,4'-biphenylenedi...	360	C26H20N2	006311-48-4	91
2			1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	60
3			Pentacyclo[18.4.1.1(2,7).1(8,13)...	360	C28H24	101077-60-5	43
4			Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	43
5			1,3,2-Dioxaborolane, bis(spiro[4...	360	C20H13B06	1000150-23-7	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050521\
Data File : BF123824.D
Acq On : 5 May 2021 13:12
Operator : JU/CG
Sample : PB136166BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB136166BL

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
Propane, 1,1-di...	2.204	3.8	ng	317257	1	6.792	1657570	20.0
2-Pentanone, 4-...	5.022	6.6	ng	543447	1	6.792	1657570	20.0
Dibenzylidene 4...	16.774	6.6	ng	572160	6	15.427	1739690	20.0