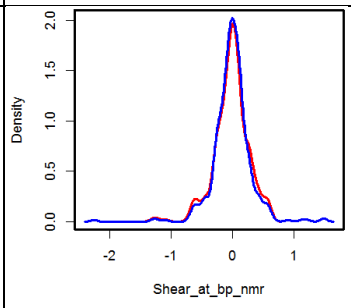
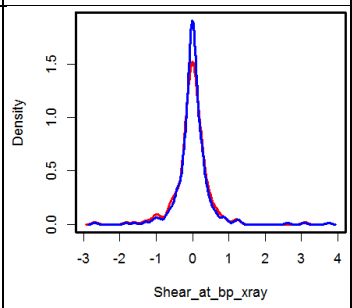
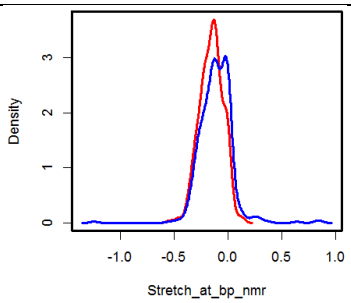
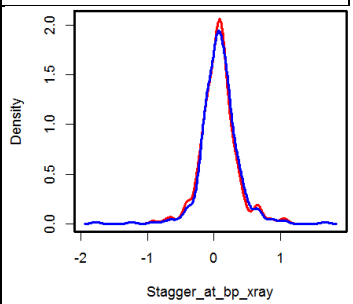
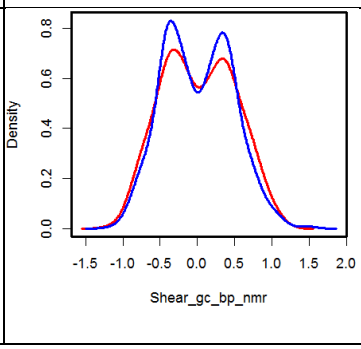
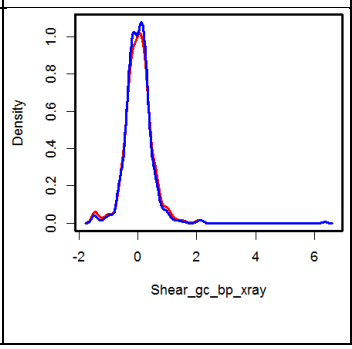
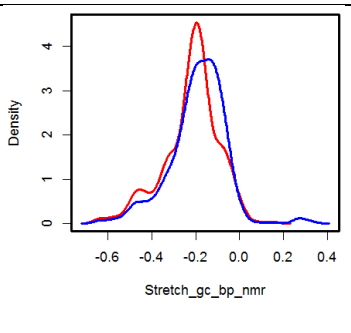
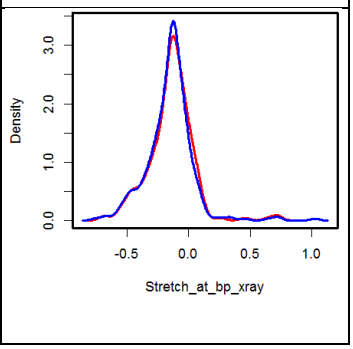
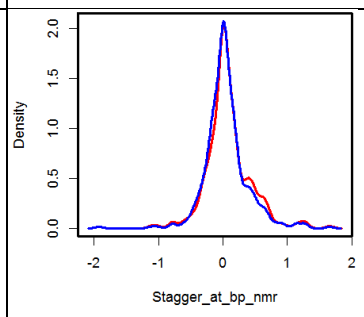
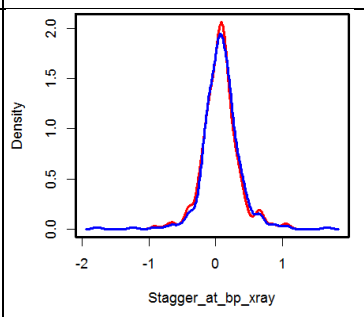
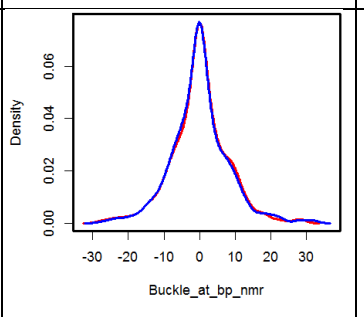
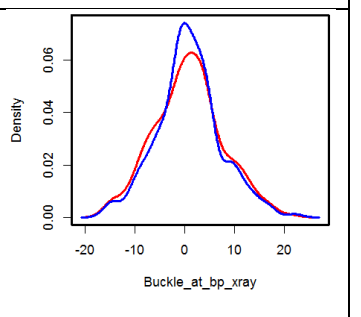
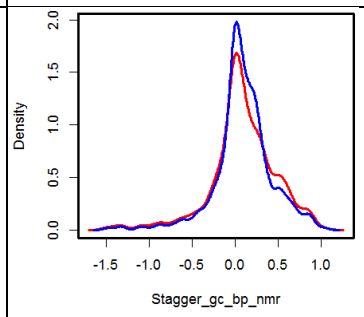
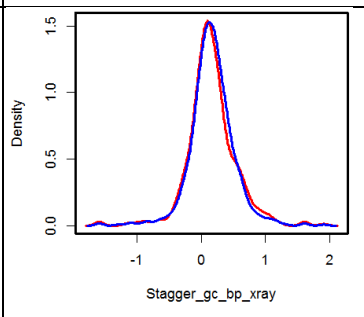
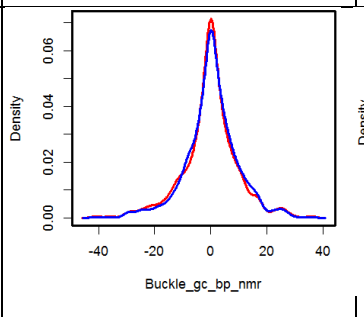
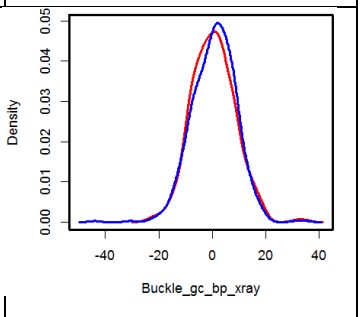
# Analysis of B-DNA, A-RNA and DNA-RNA hybrid structures deposited in PDB server

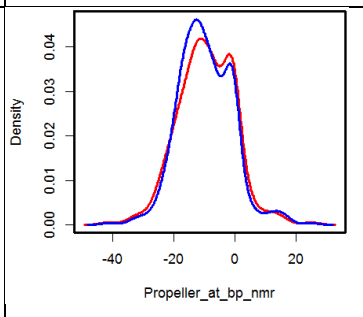
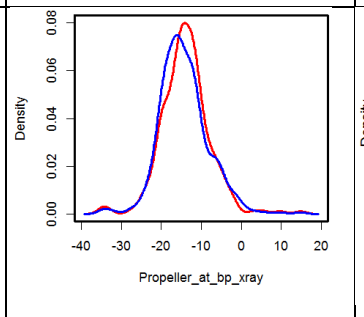
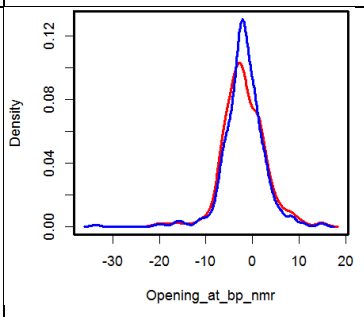
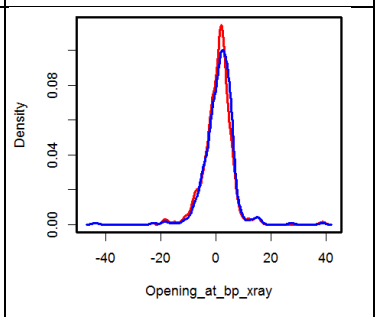
All B-DNA, A-RNA and DNA-RNA hybrid structures deposited in PDB server are analyzed to derive base pair and base pair step parameters using the method described in Patro *et al* (Accepted for publication in JMB). Unusual conformations (such as loop, quadruple *etc*) containing structures are not considered for the analysis. Table 1 (A-C) contains density plots corresponding to 12 base pair and base pair step parameters derived for DNA, RNA and DNA-RNA hybrid duplex structures with (blue) and without (red) modified nucleotides or ligands. It can be clearly seen from these plots that the range adopted by the 12 parameters does not differ significantly between these two cases. Thus, for average and standard deviations [1] calculations of base pair and base pair step parameters, duplexes with modified nucleotides or ligands are also considered. These values are subsequently used in the sequence specific modeling of DNA/RNA/DNA-RNA hybrid duplexes in 3D-NuS.

**Table 1(A). Density plots for all base pair and base pair step parameters of B-DNA**

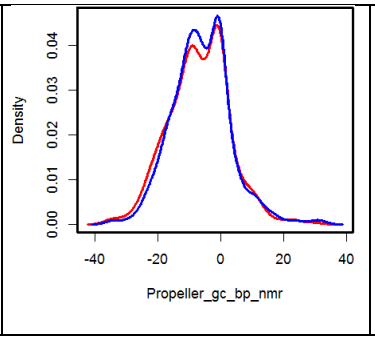
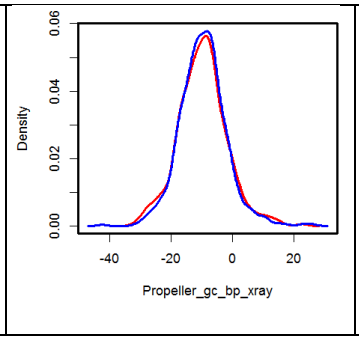
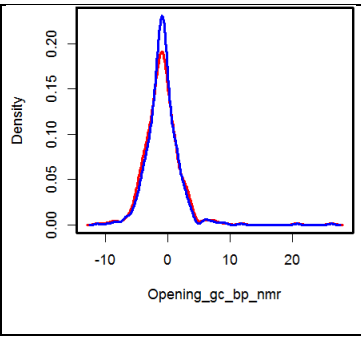
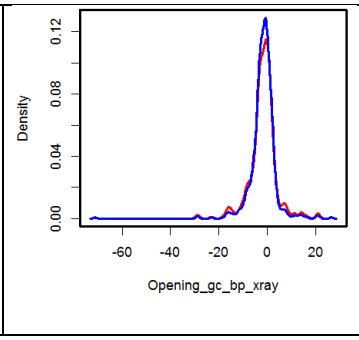
| Base pair | **Shear** | | **Stretch** | |
|---|---|---|---|---|
| | **NMR** | **X-Ray** | **NMR** | **X-Ray** |
| **A-T** |  |  |  |  |
| **G-C** |  |  |  |  |

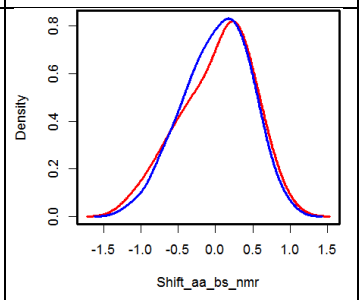
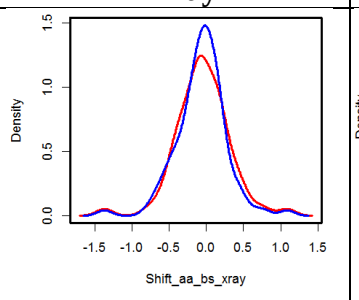
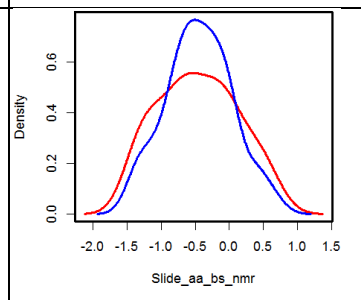
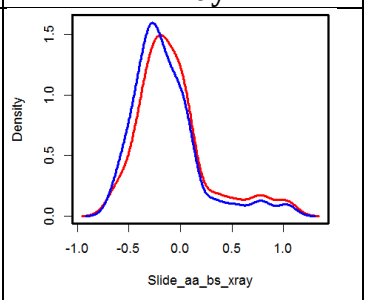
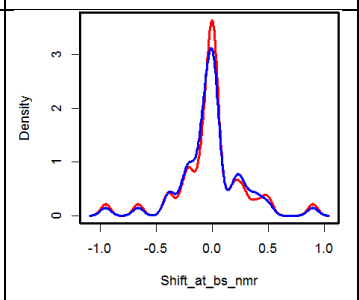
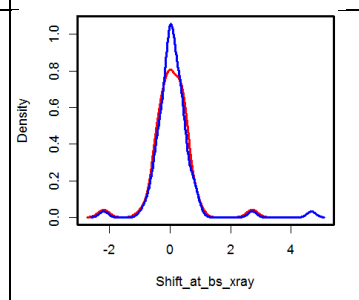
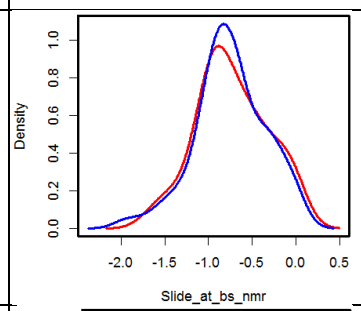
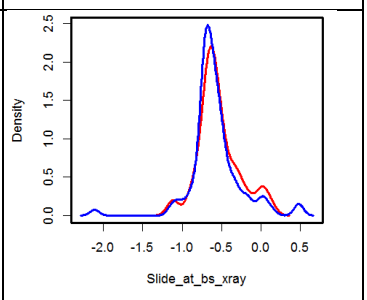
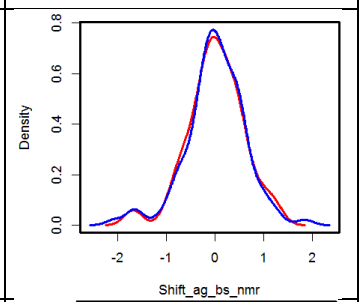
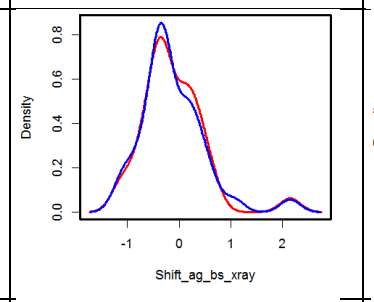
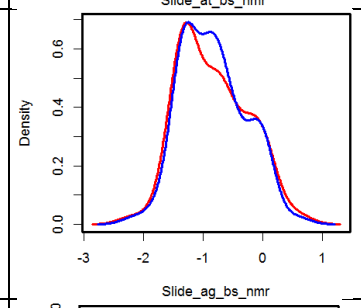
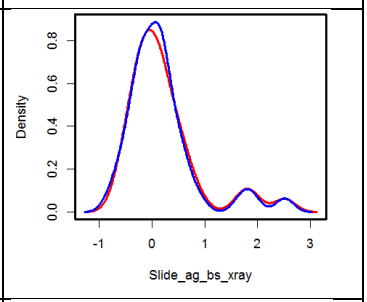
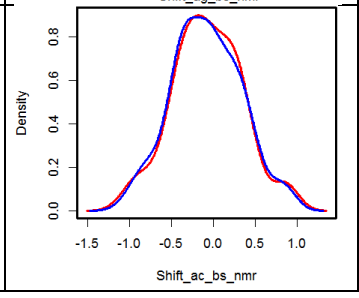
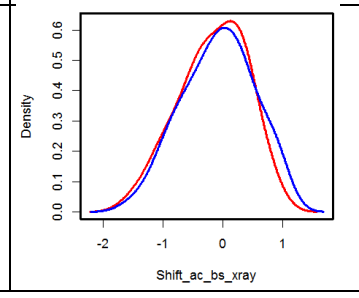
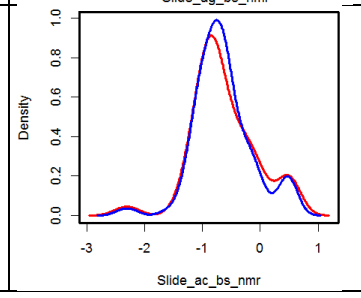
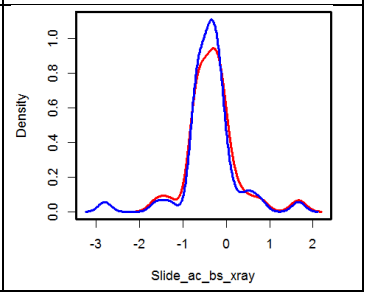
Continue…

| Base pair | Stagger | | Buckle | |
|---|---|---|---|---|
| | **NMR** | **X-Ray** | **NMR** | **X-Ray** |
| **A-T** |  |  |  |  |
| **G-C** |  |  |  |  |

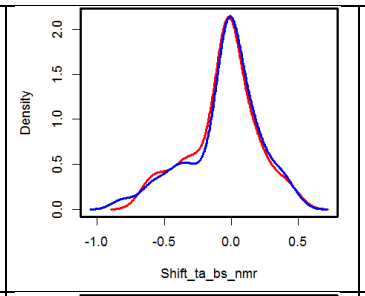
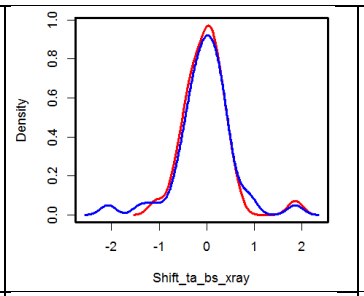
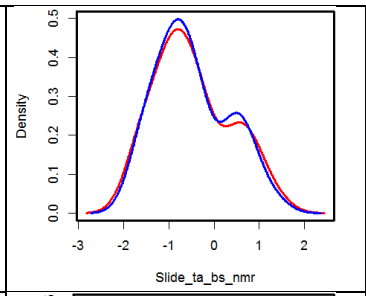
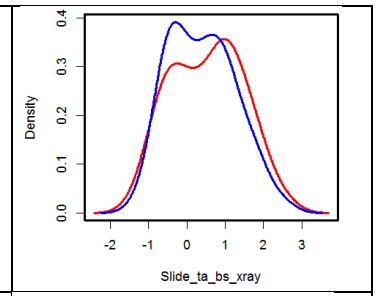
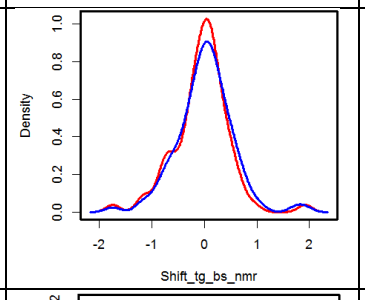
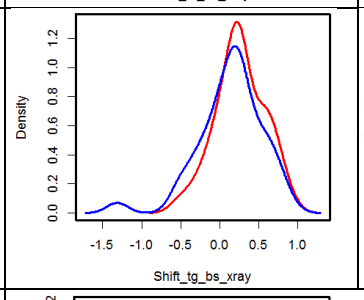
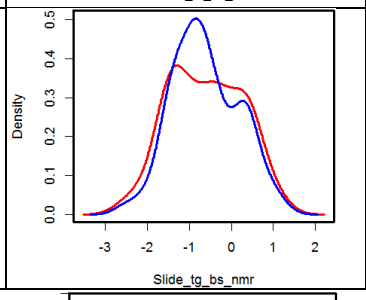
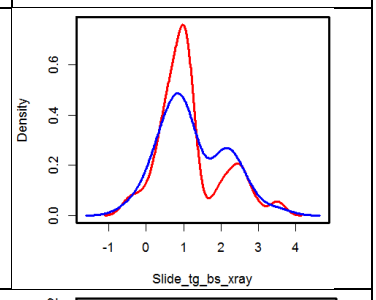
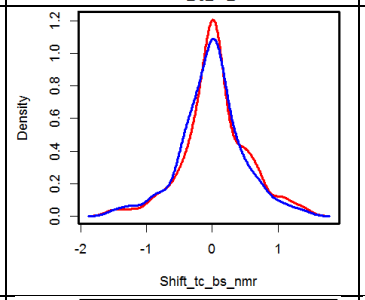
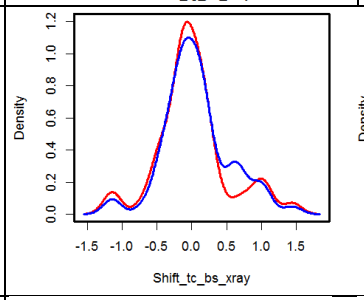
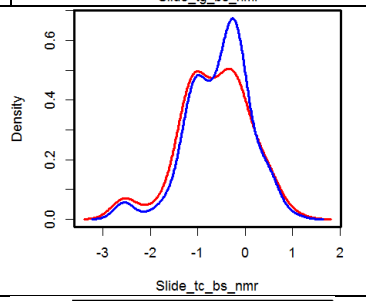
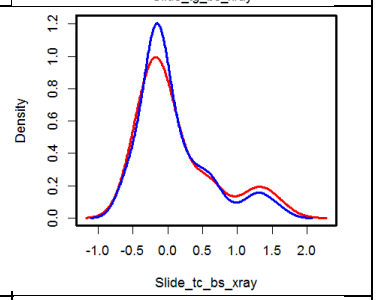
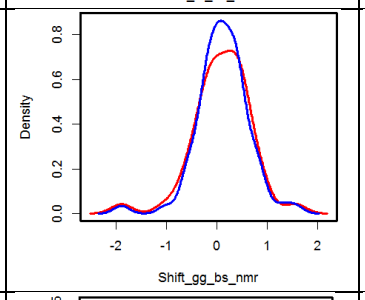
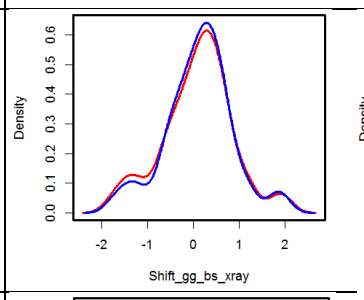
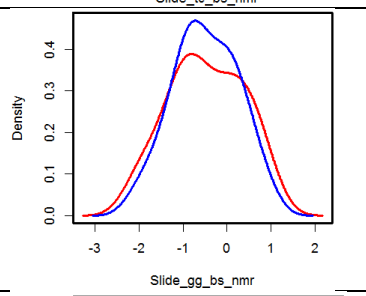
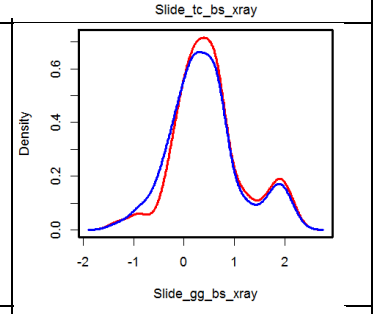
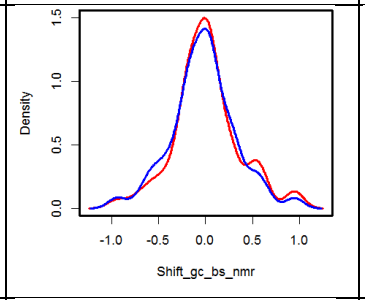
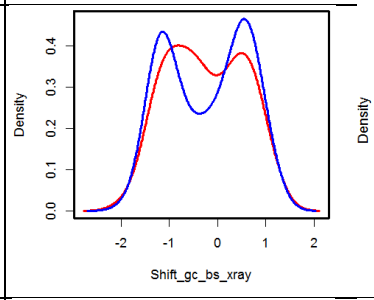
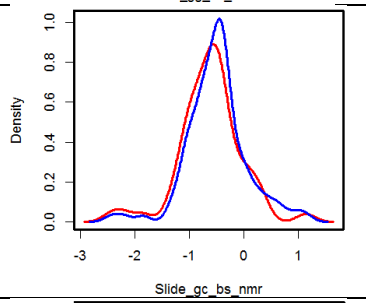
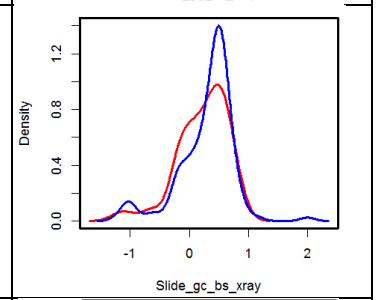
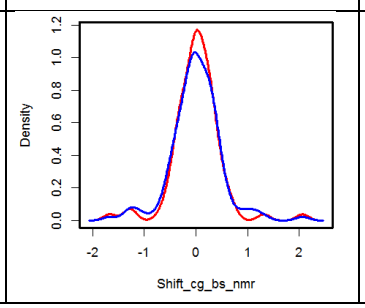
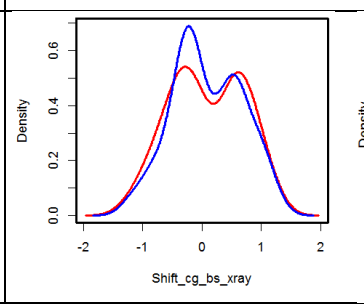
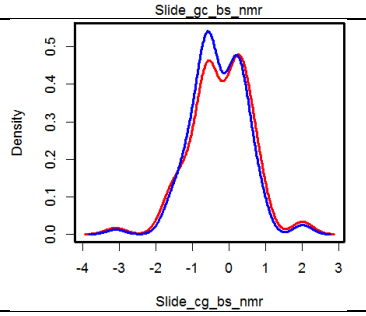
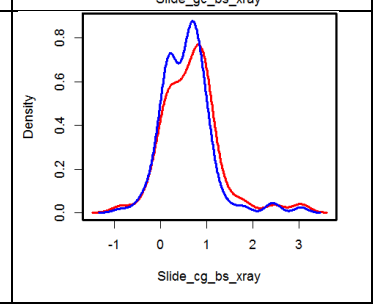
| Base pair | Propeller | | Opening | |
|---|---|---|---|---|
| | **NMR** | **X-Ray** | **NMR** | **X-Ray** |
| **A-T** |  |  |  |  |

Continue…

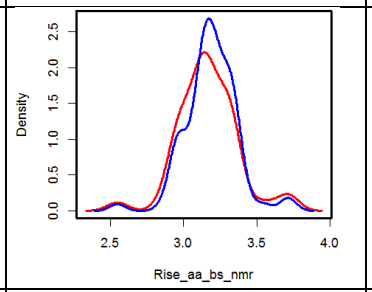
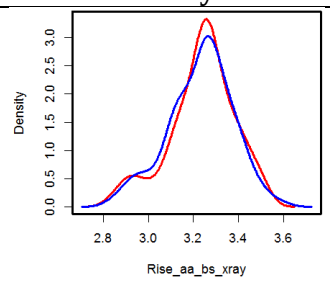
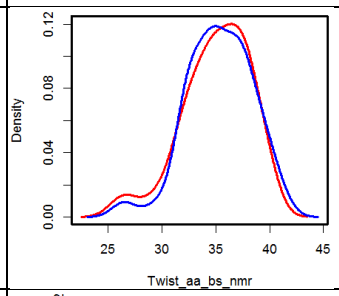
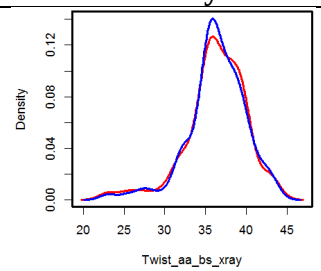
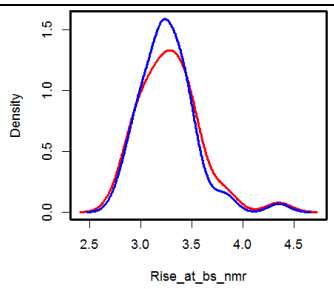
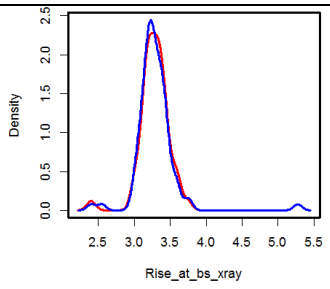
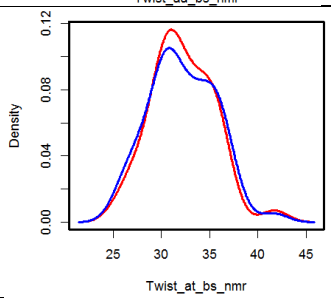
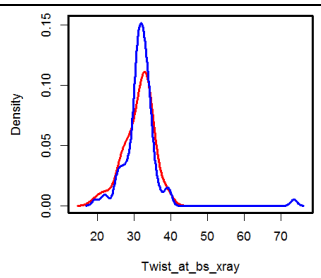
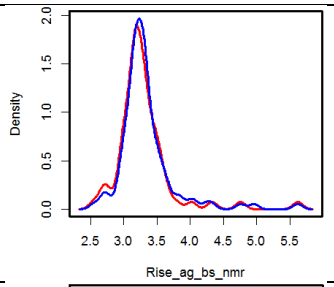
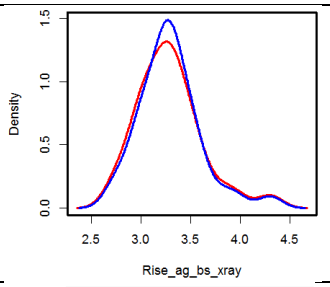
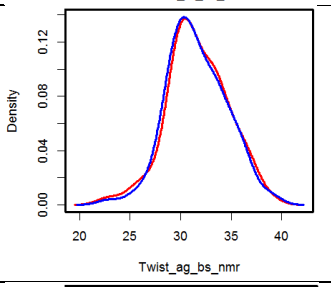
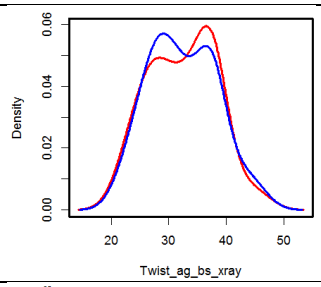
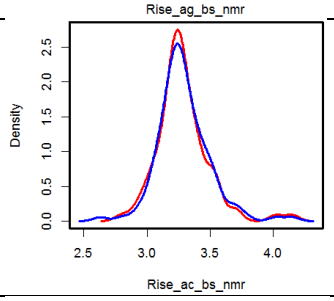
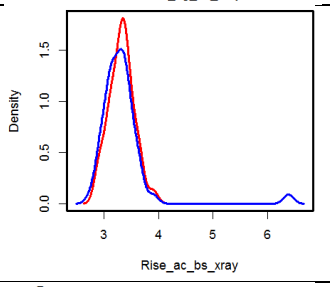
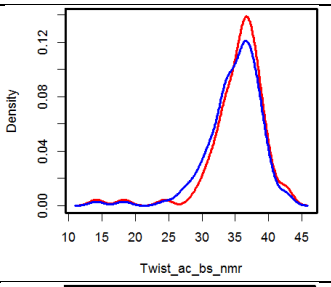
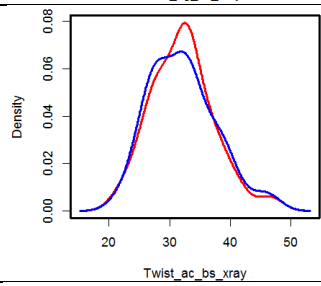
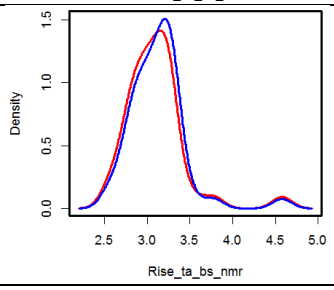
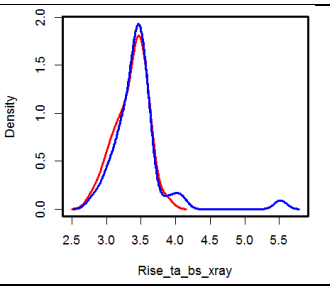
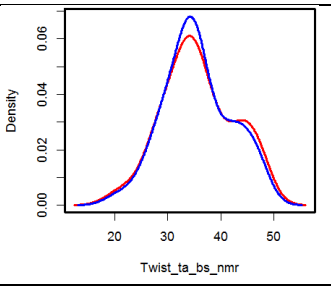
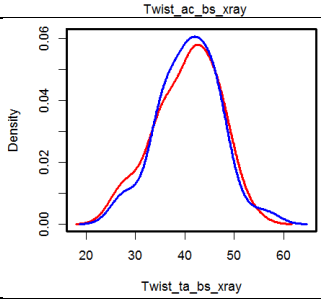
| | | | | |
|---|---|---|---|---|
| **G-C** |  |  |  |  |

| Base pair step | **Shift** | | **Slide** | |
|---|---|---|---|---|
| | **NMR** | **X-Ray** | **NMR** | **X-Ray** |
| **AA** |  |  |  |  |
| **AT** |  |  |  |  |
| **AG** |  |  |  |  |
| **AC** |  |  |  |  |

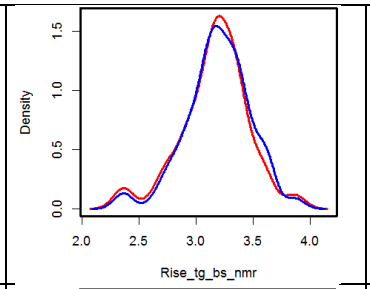
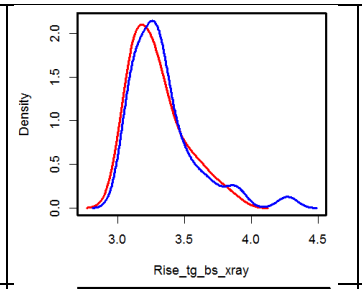
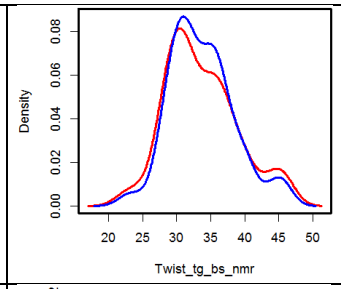
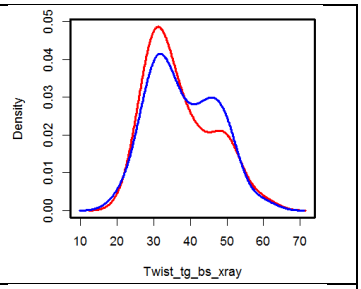
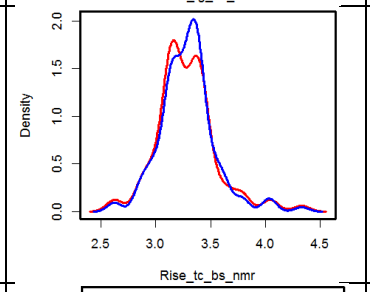
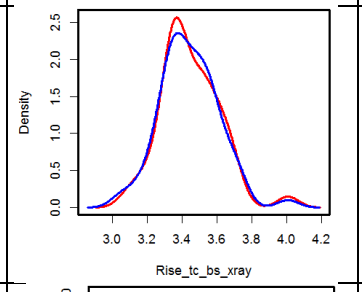
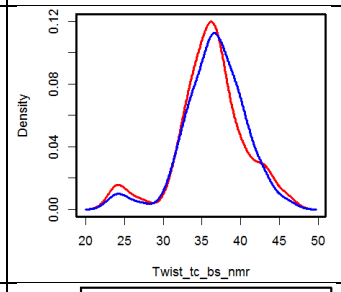
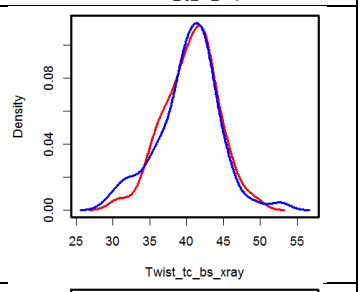
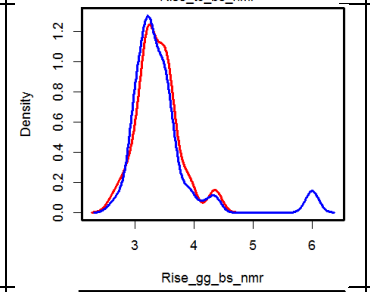
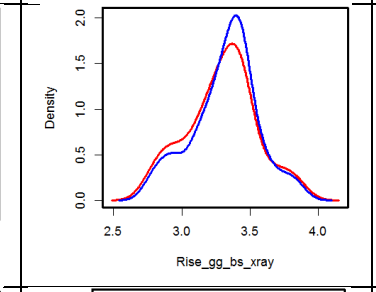
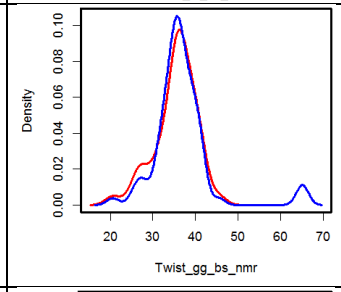
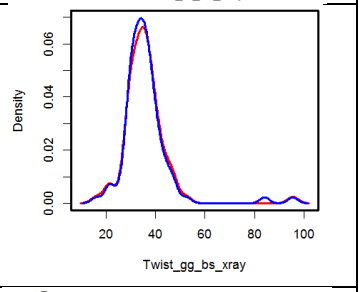
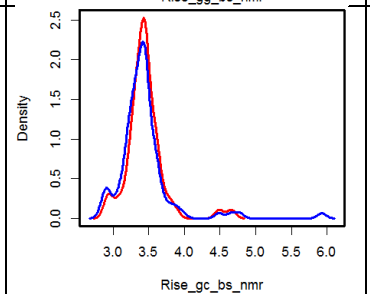
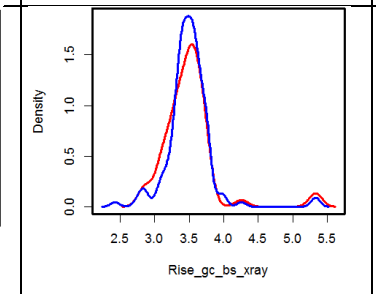
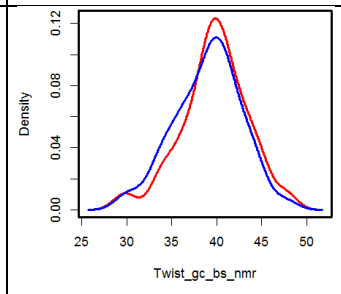
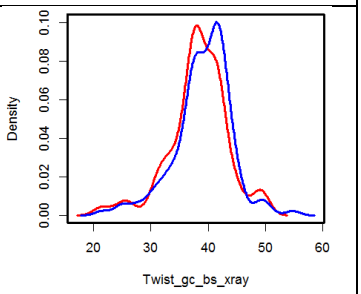
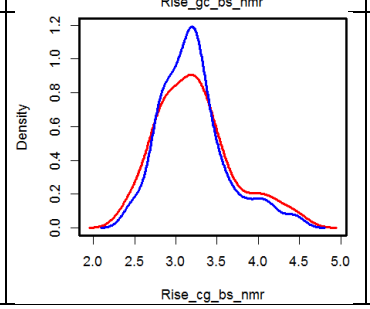
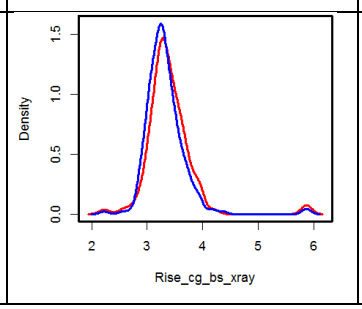
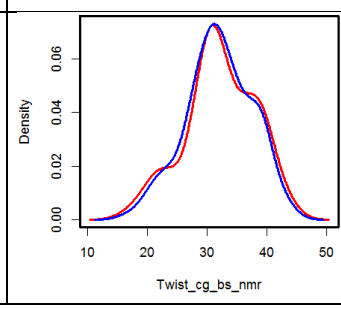
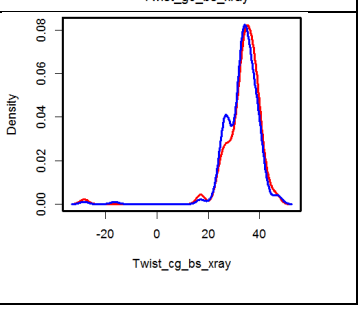
Continue…

| | | | | |
|---|---|---|---|---|
| **TA** |  |  |  |  |
| **TG** |  |  |  |  |
| **TC** |  |  |  |  |
| **GG** |  |  |  |  |
| **GC** |  |  |  |  |
| **CG** |  |  |  |  |

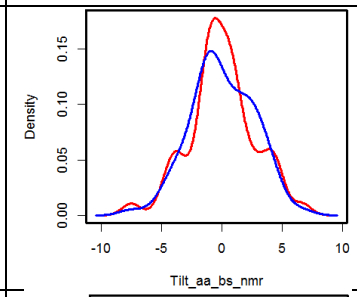
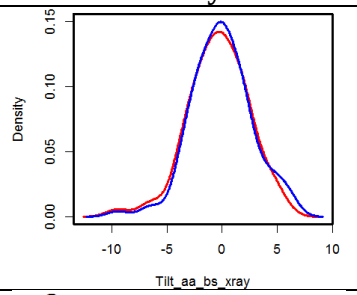
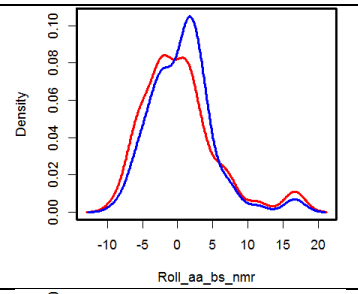
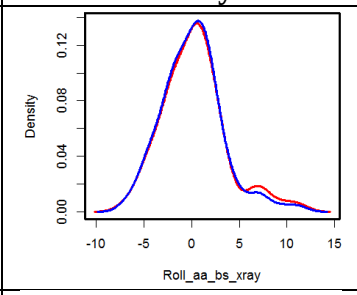
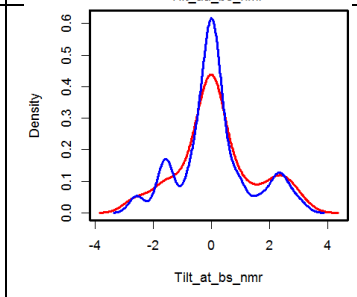
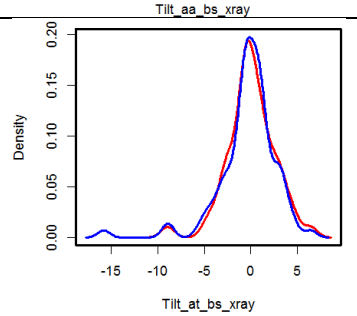
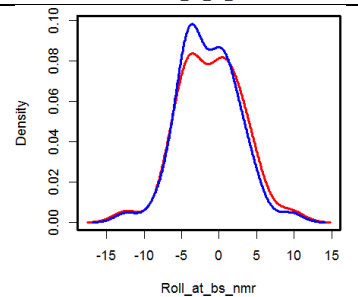
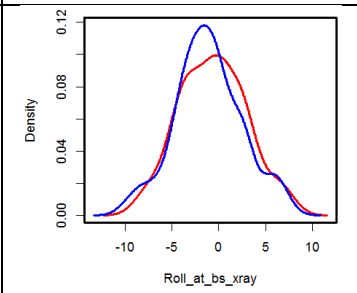
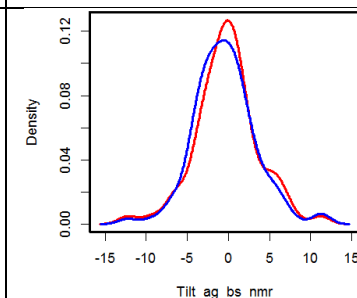
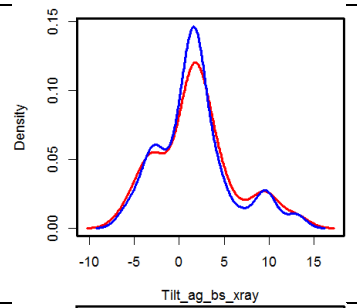
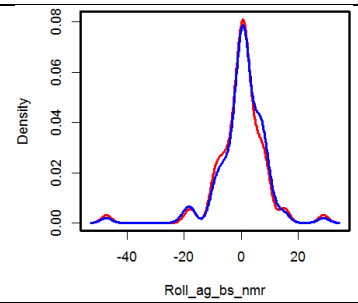
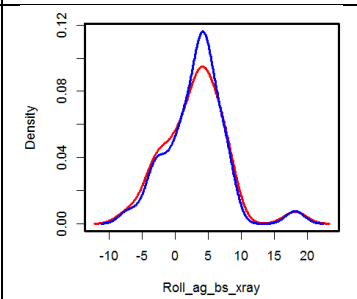
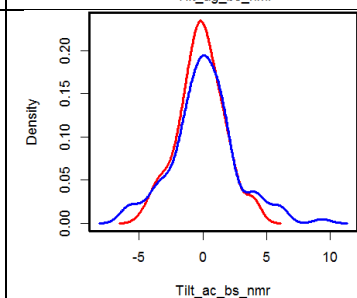
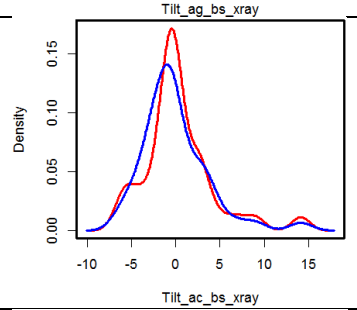
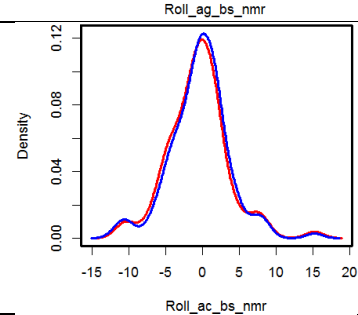
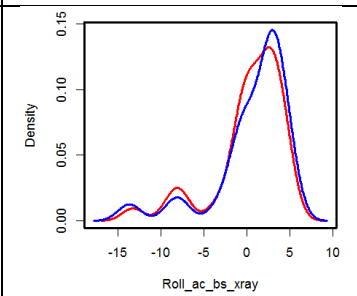
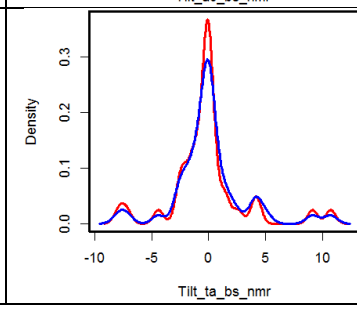
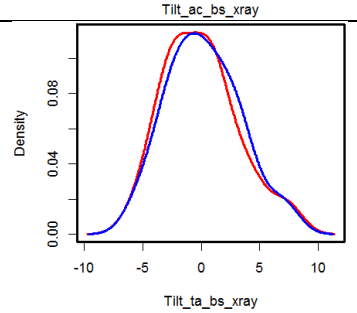
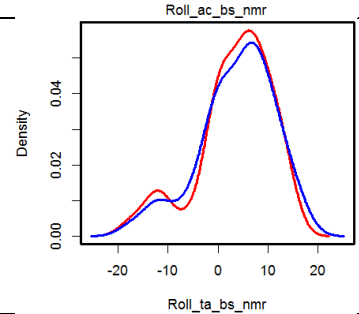
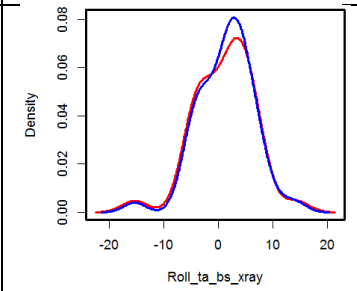
Continue…

| Base pair step | Rise | | Twist | |
|---|---|---|---|---|
| | NMR | X-Ray | NMR | X-Ray |
| **AA** |  |  |  |  |
| **AT** |  |  |  |  |
| **AG** |  |  |  |  |
| **AC** |  |  |  |  |
| **TA** |  |  |  |  |

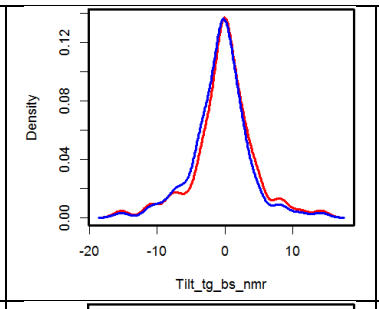
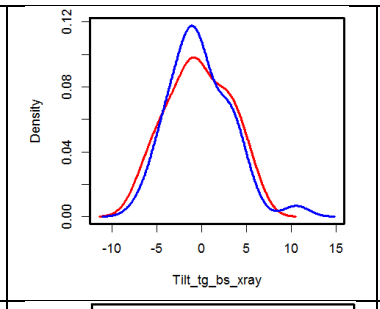
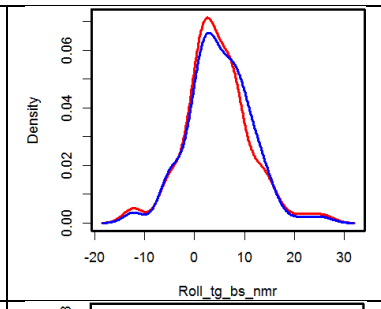
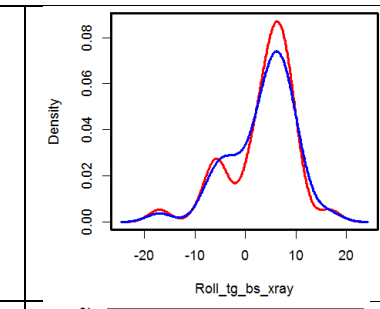
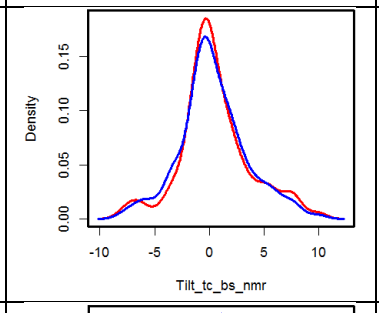
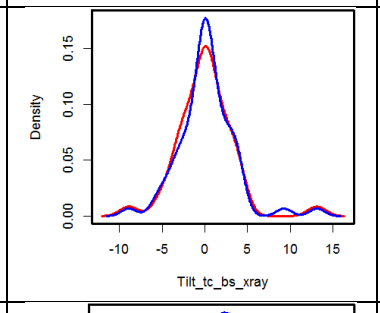
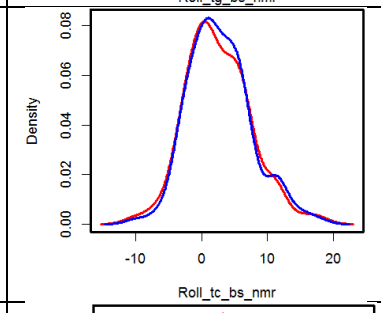
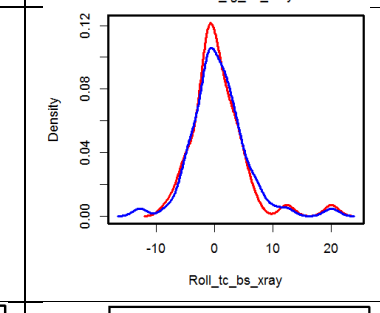
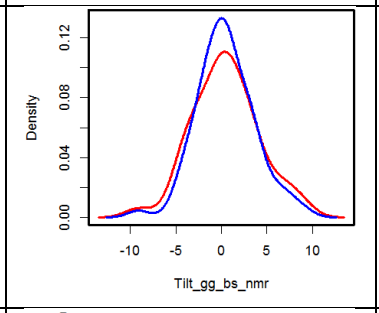
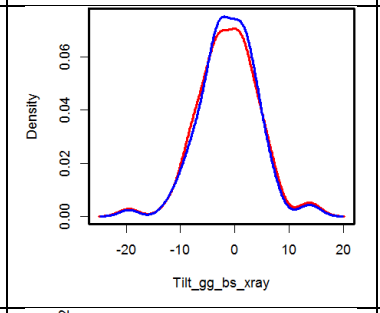
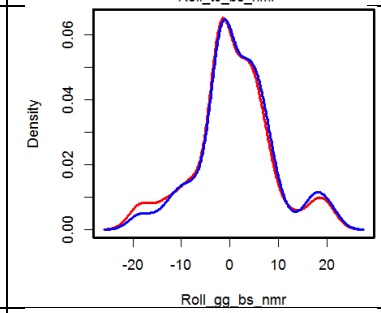
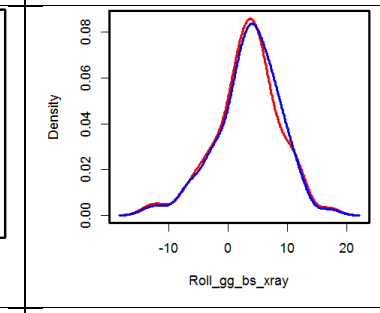
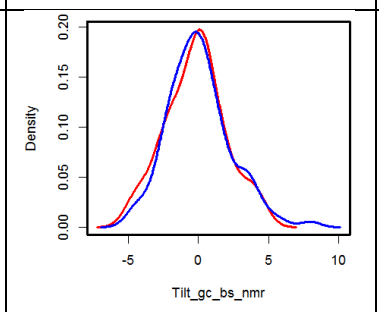
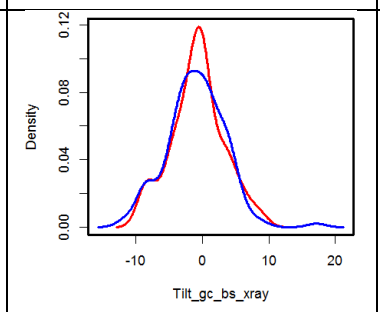
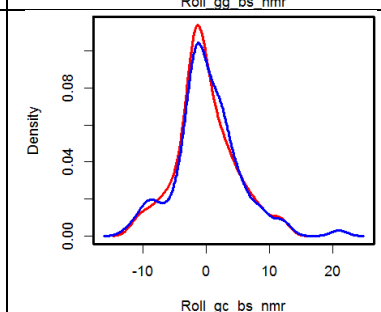
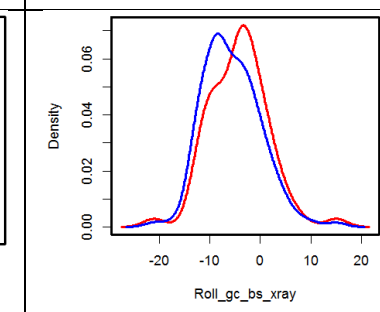
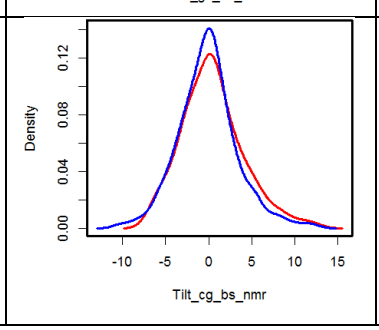
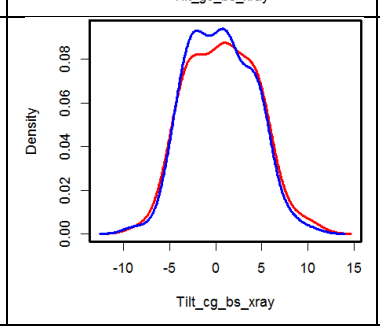
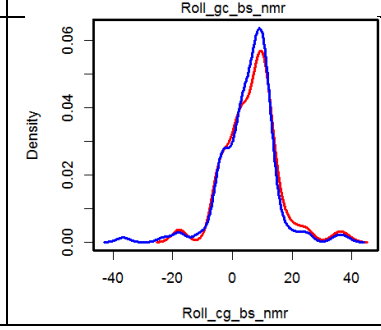
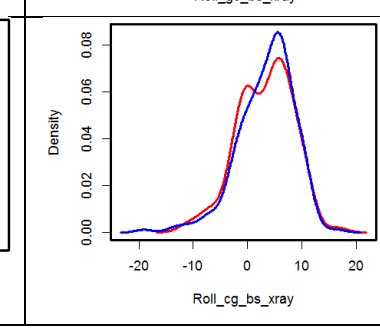
Continue…

| | | | | |
|---|---|---|---|---|
| **TG** |  |  |  |  |
| **TC** |  |  |  |  |
| **GG** |  |  |  |  |
| **GC** |  |  |  |  |
| **CG** |  |  |  |  |

Continue…

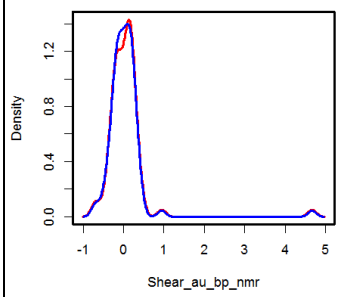
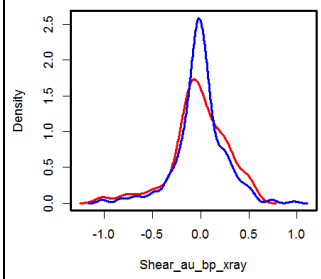
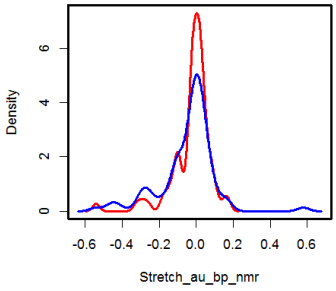
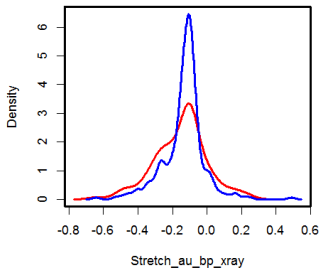
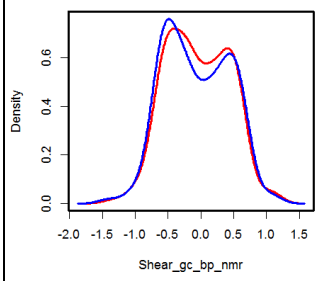
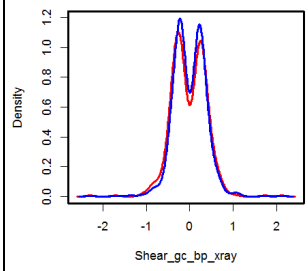
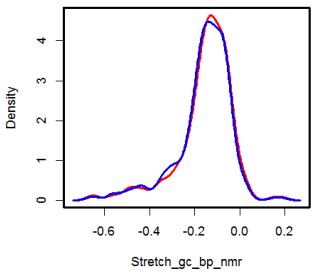
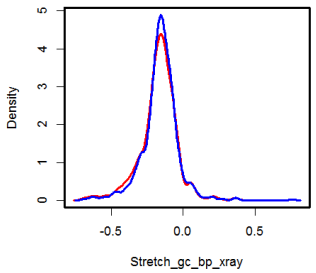
| Base pair step | Tilt | | Roll | |
|---|---|---|---|---|
| | NMR | X-Ray | NMR | X-Ray |
| **AA** |  |  |  |  |
| **AT** |  |  |  |  |
| **AG** |  |  |  |  |
| **AC** |  |  |  |  |
| **TA** |  |  |  |  |

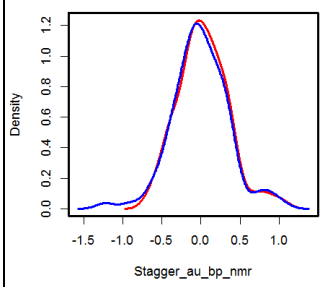
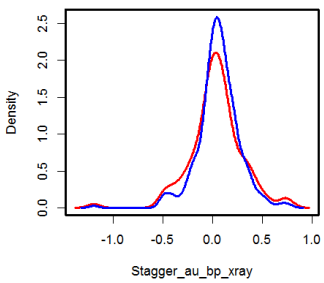
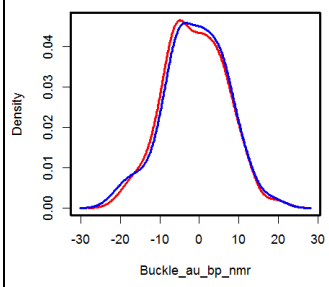
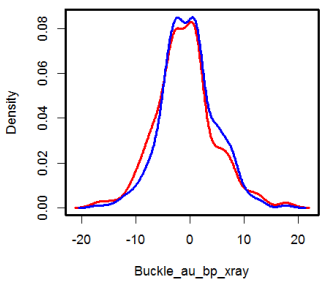
Continue…

| | | | | |
|---|---|---|---|---|
| **TG** |  |  |  |  |
| **TC** |  |  |  |  |
| **GG** |  |  |  |  |
| **GC** |  |  |  |  |
| **CG** |  |  |  |  |

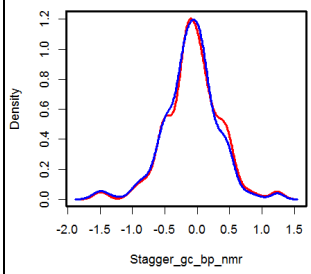
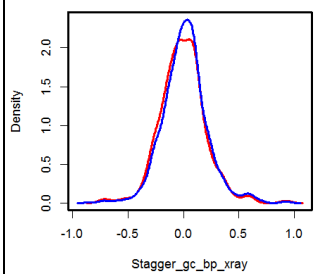
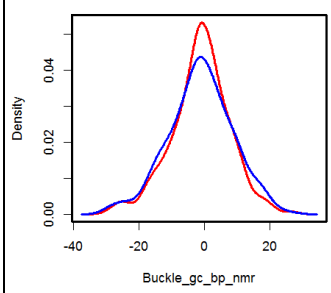
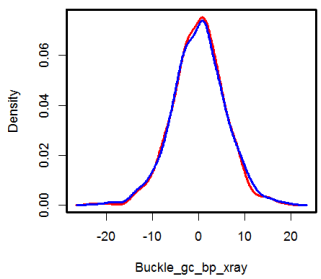
Continue…

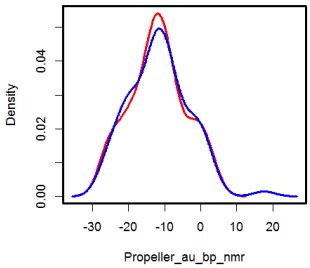
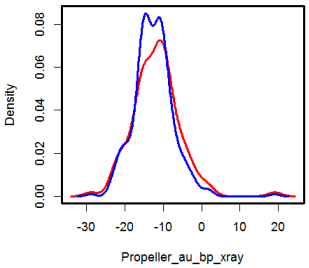
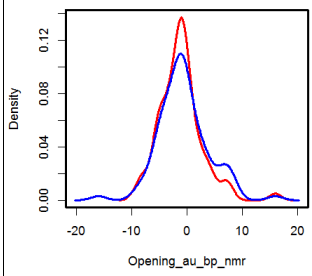
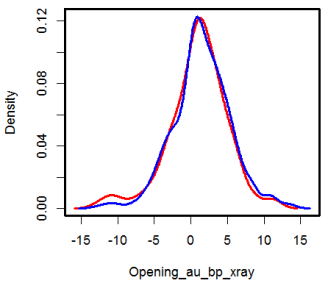
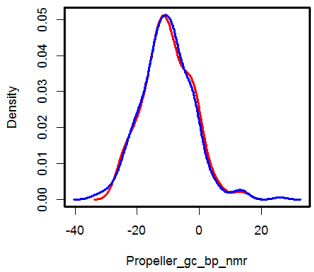
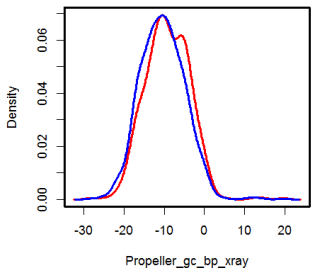
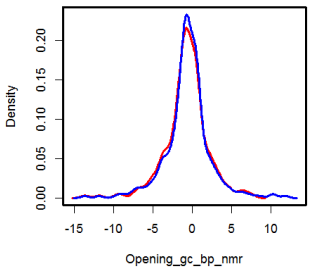
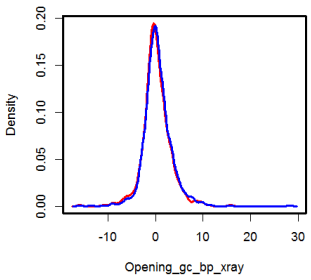
**Table 1(B). Density plots for all base pair and base pair step parameters of A-RNA**

| Base pair | Shear | | Stretch | |
|---|---|---|---|---|
| | **NMR** | **X-Ray** | **NMR** | **X-Ray** |
| **A-U** |  |  |  |  |
| **G-C** |  |  |  |  |

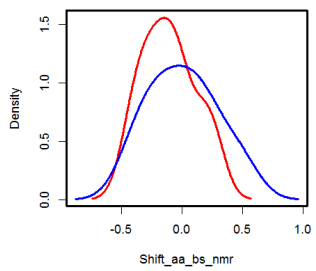
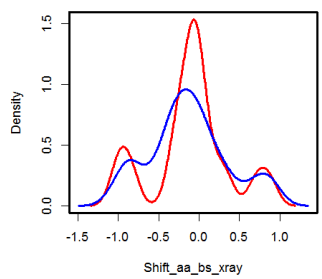
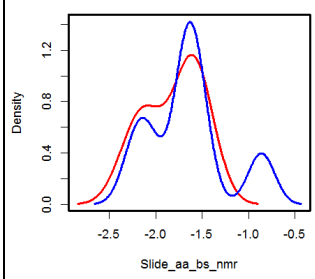
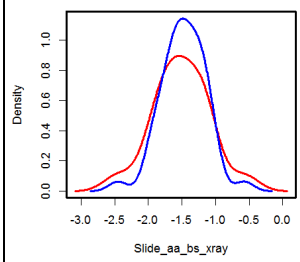
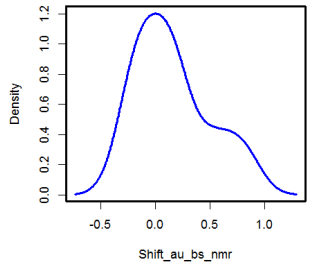
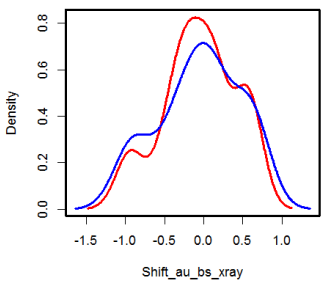
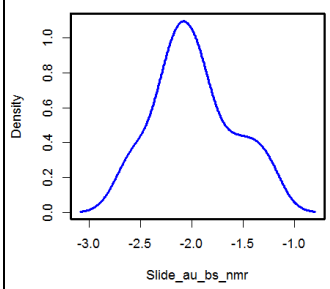
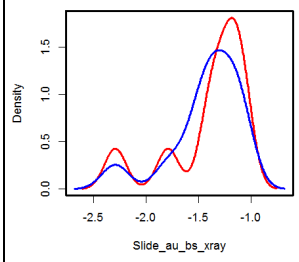
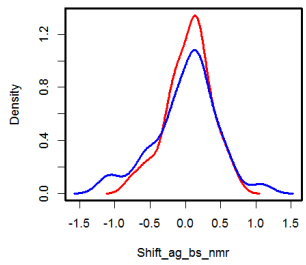
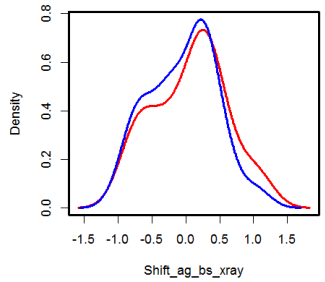
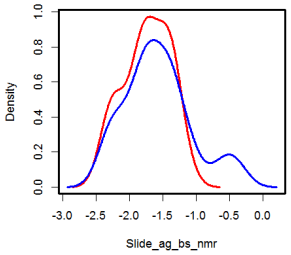
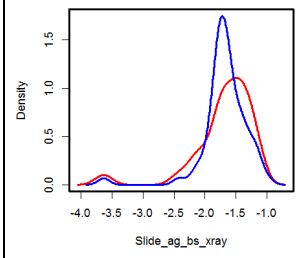
| Base pair | Stagger | | Buckle | |
|---|---|---|---|---|
| | **NMR** | **X-Ray** | **NMR** | **X-Ray** |
| **A-U** |  |  |  |  |

Continue…

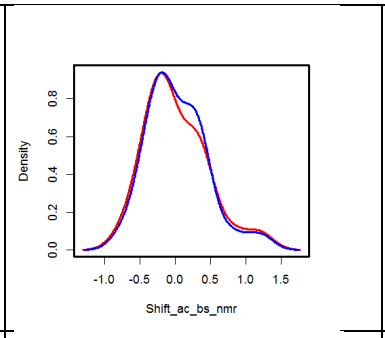
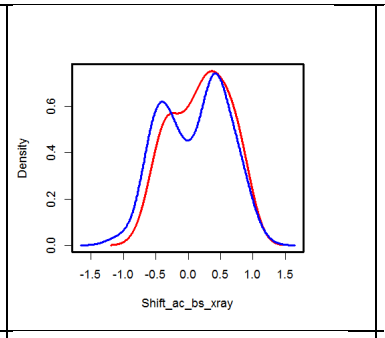
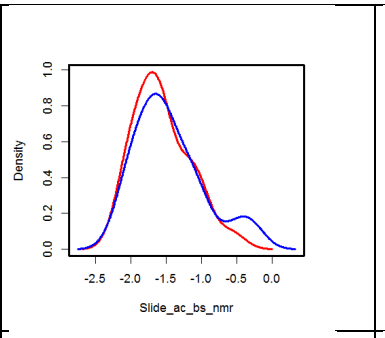
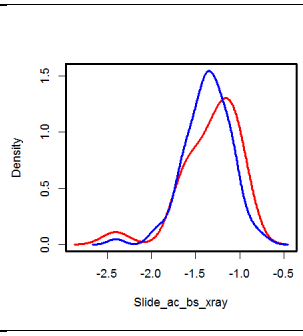
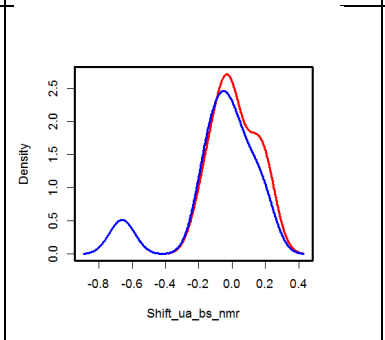
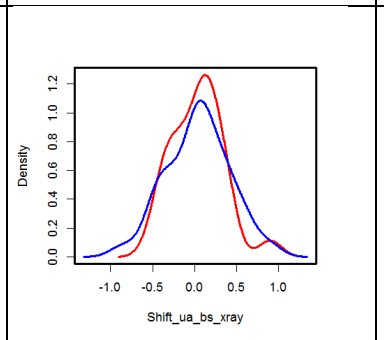
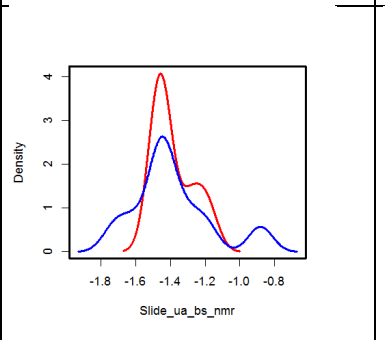
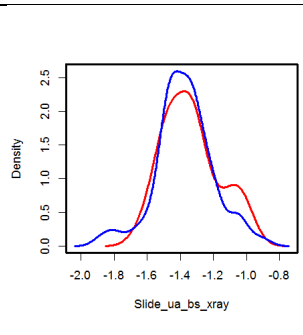
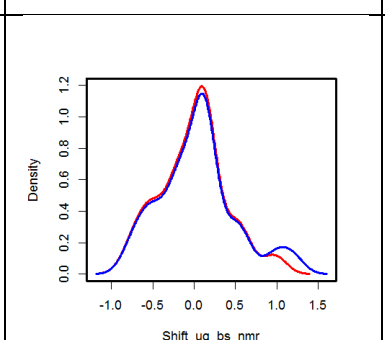
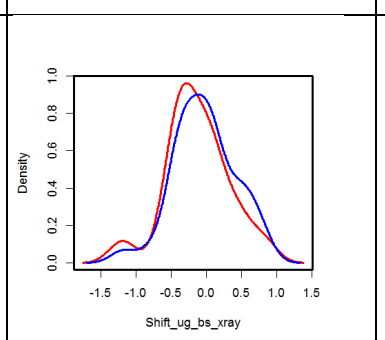
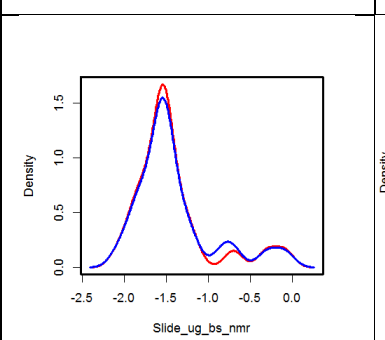
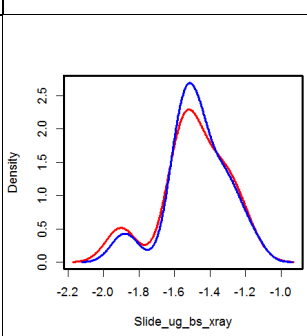
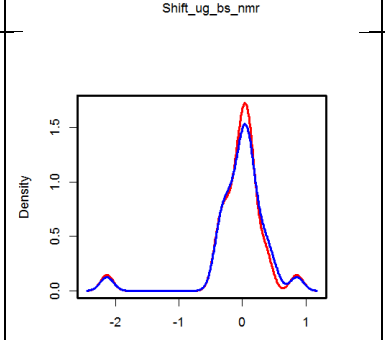
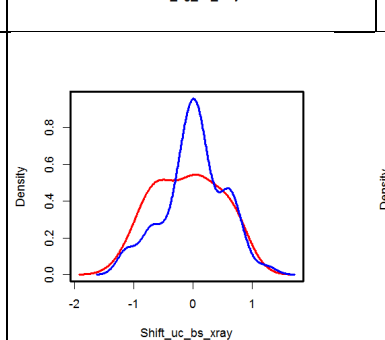
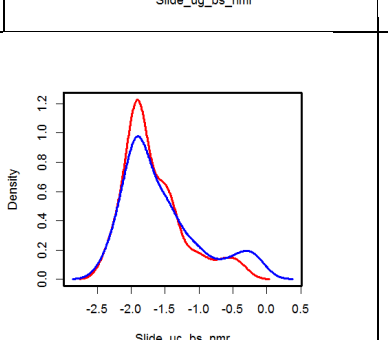
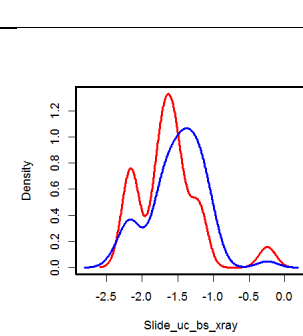
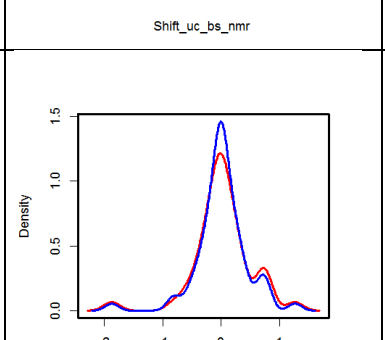
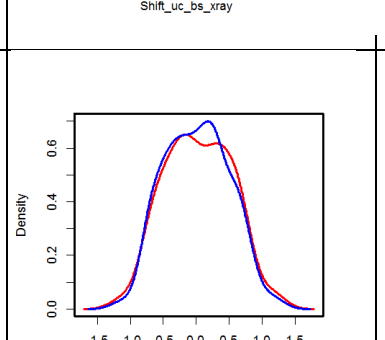
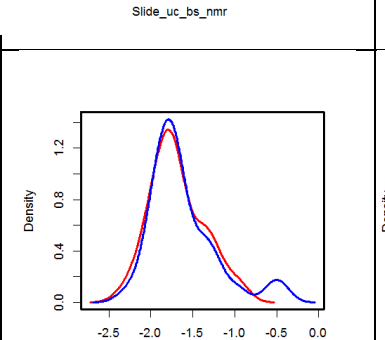
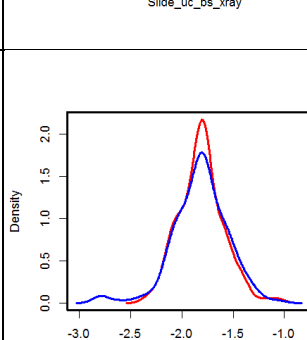
| | | | | |
|---|---|---|---|---|
| **G-C** |  |  |  |  |

| Base pair | **Propeller** | | **Opening** | |
|---|---|---|---|---|
| | **NMR** | **X-Ray** | **NMR** | **X-Ray** |
| **A-U** |  |  |  |  |
| **G-C** |  |  |  |  |

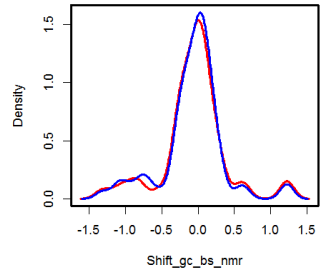
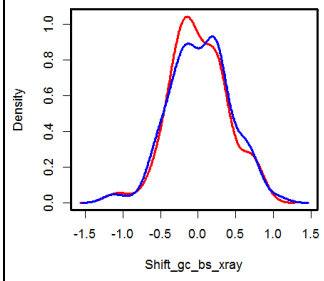
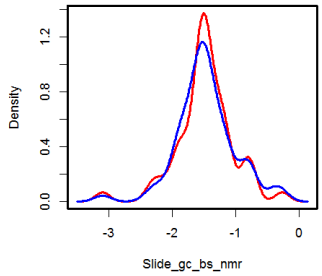
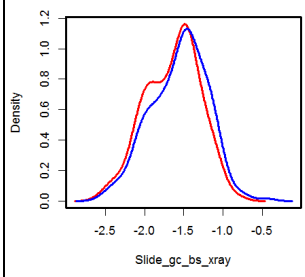
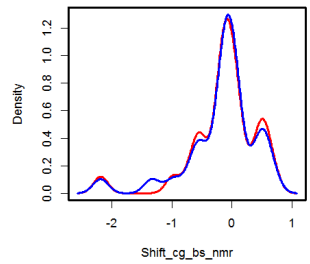
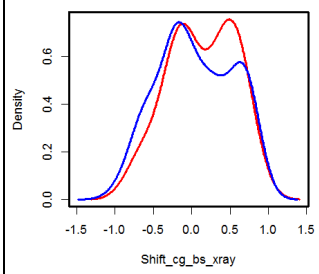
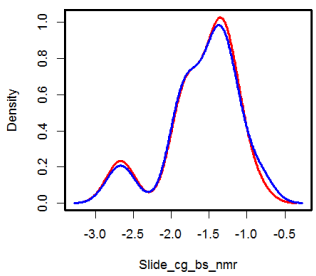
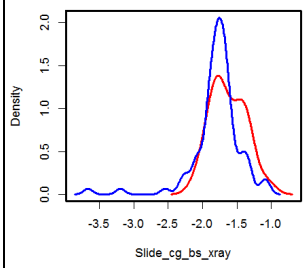
Continue…

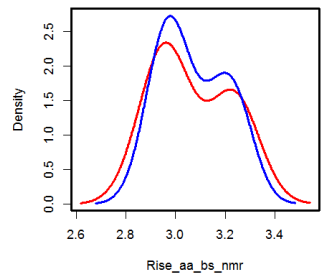
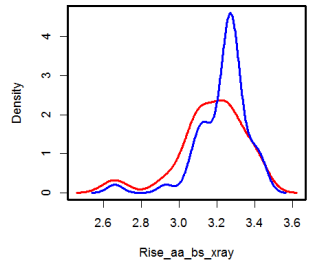
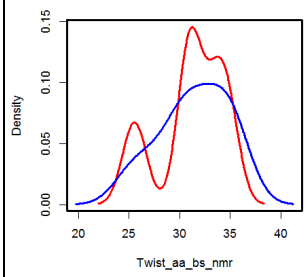
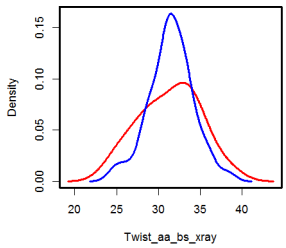
| Base pair step | Shift | | Slide | |
|---|---|---|---|---|
| | **NMR** | **X-Ray** | **NMR** | **X-Ray** |
| **AA** |  |  |  |  |
| **AU** |  |  |  |  |
| **AG** |  |  |  |  |

Continue…

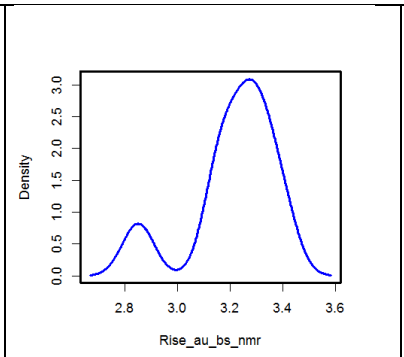
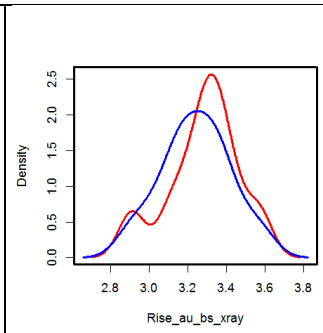
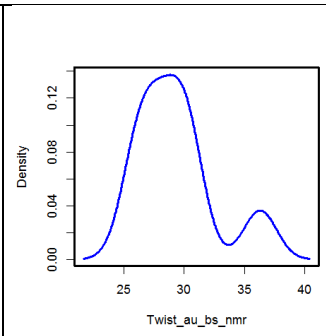
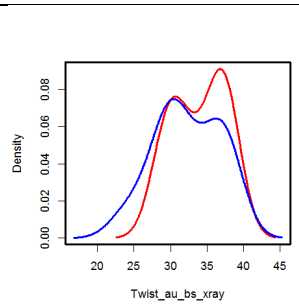
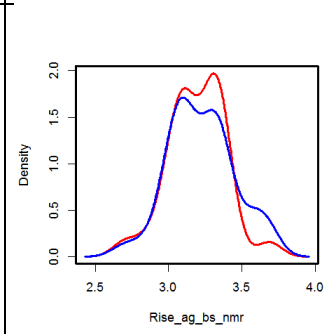
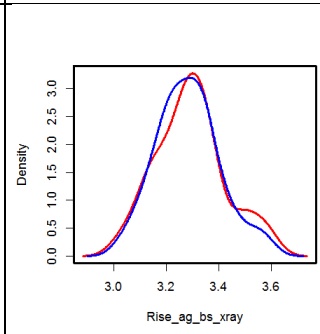
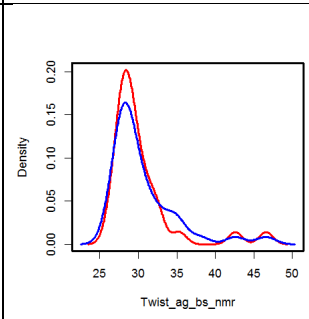
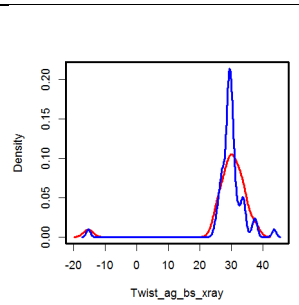
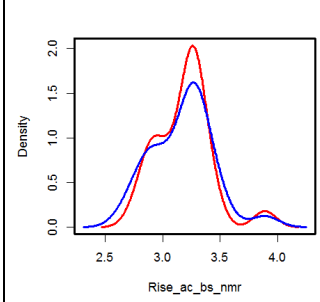
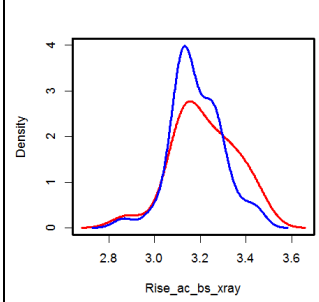
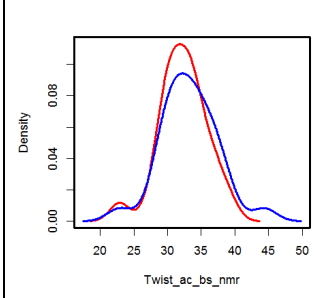
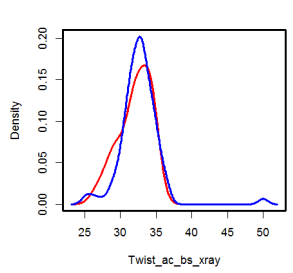
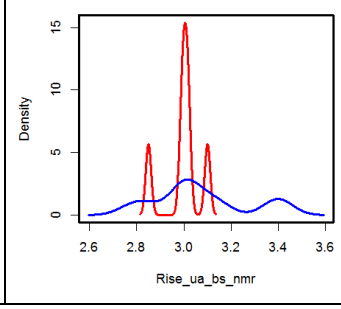
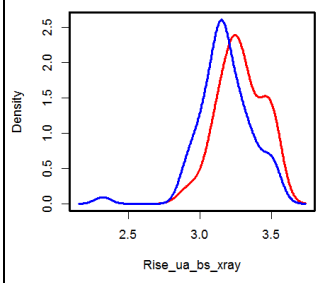
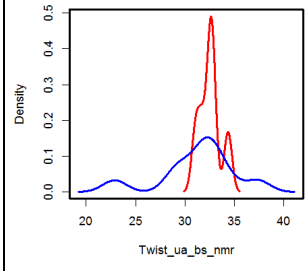
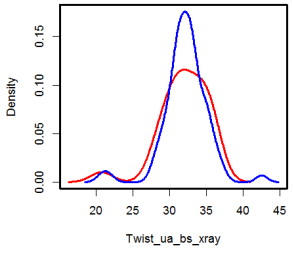
| | | | | |
|---|---|---|---|---|
| **AC** |  |  |  |  |
| **UA** |  |  |  |  |
| **UG** |  |  |  |  |
| **UC** |  |  |  |  |
| **GG** |  |  |  |  |

Continue…

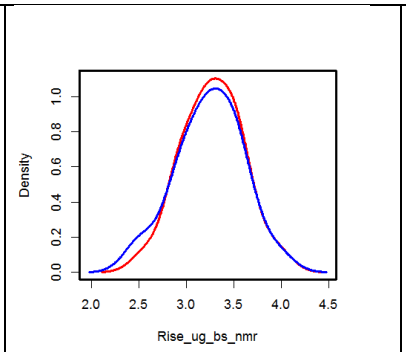
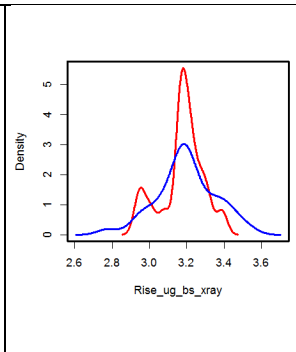
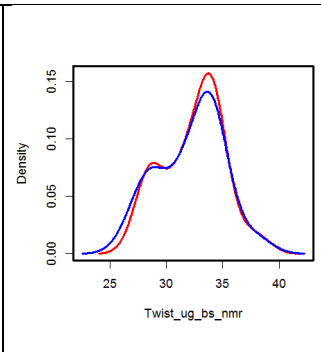
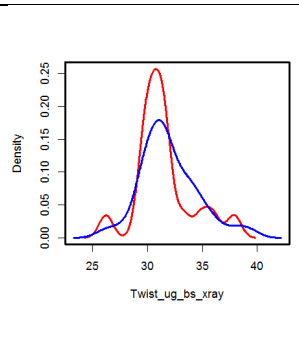
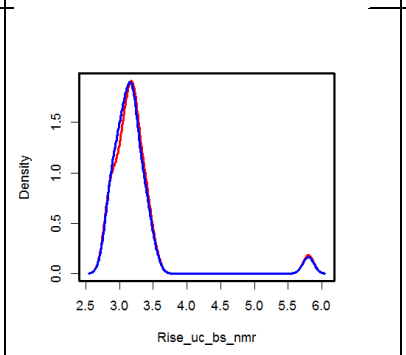
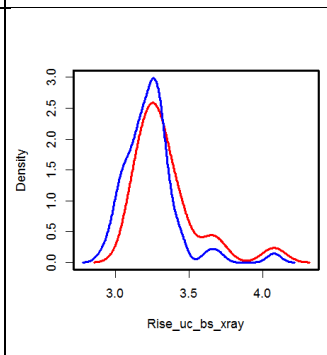
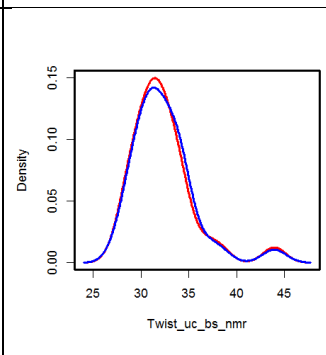
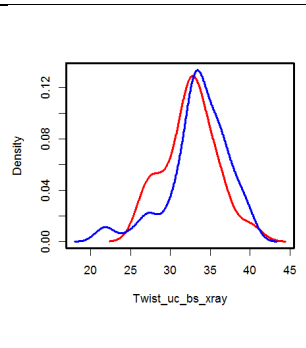
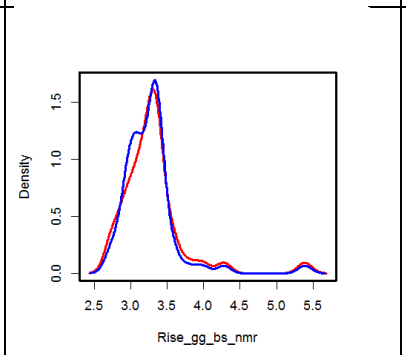
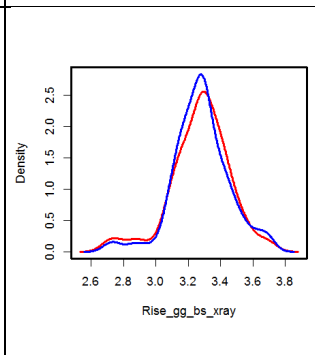
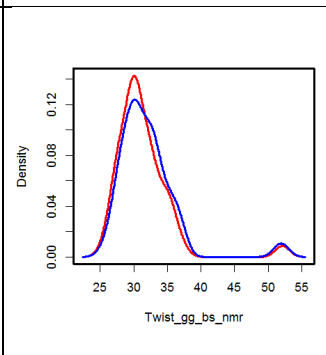
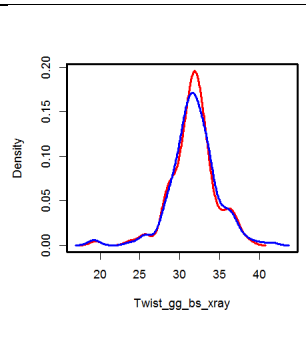
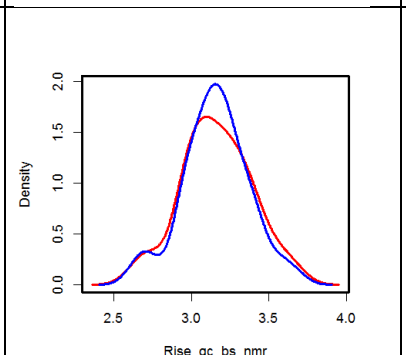
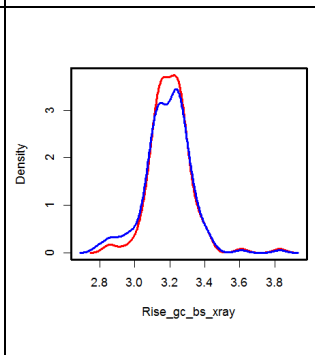
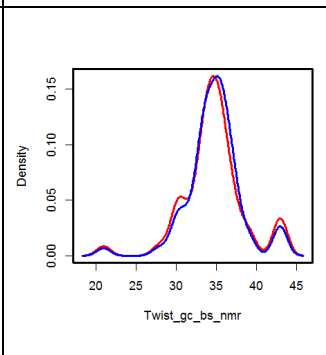
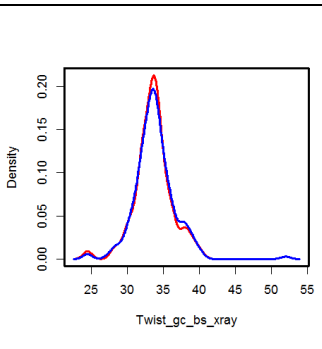
| | | | | |
|---|---|---|---|---|
| **GC** |  |  |  |  |
| **CG** |  |  |  |  |

| Base pair step | **Rise** | | **Twist** | |
|---|---|---|---|---|
| | **NMR** | **X-Ray** | **NMR** | **X-Ray** |
| **AA** |  |  |  |  |

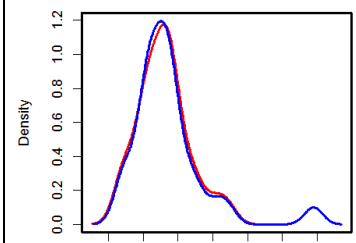
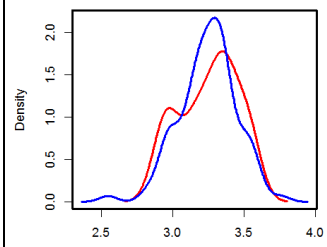
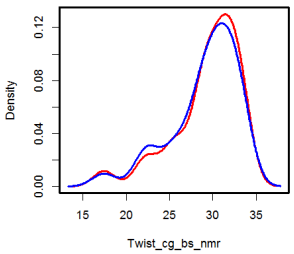
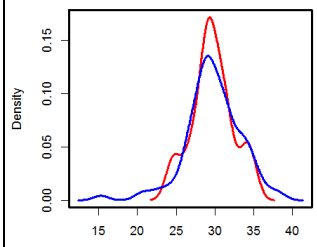
Continue…

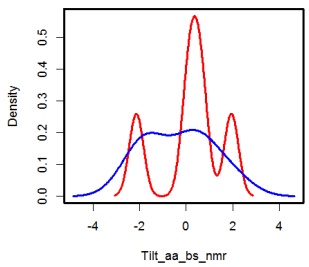
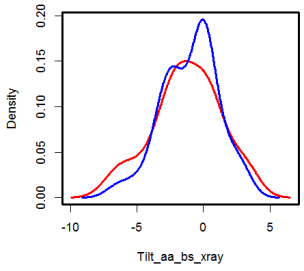
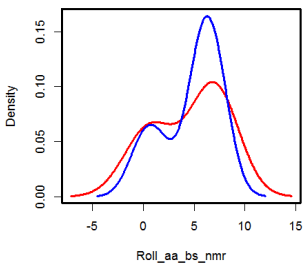
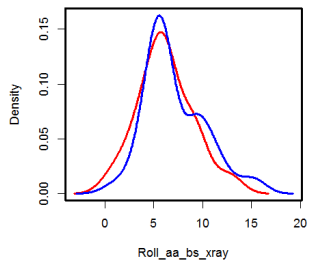
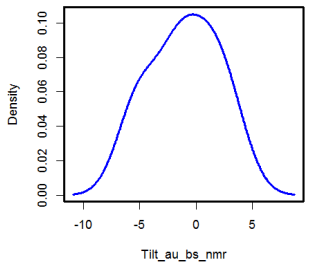
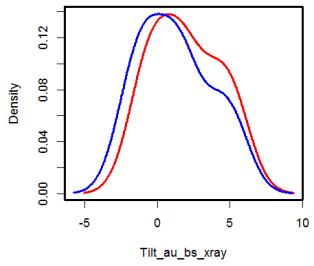
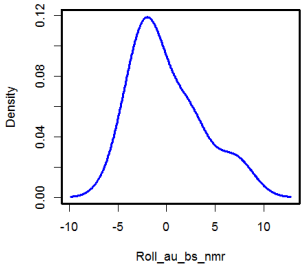
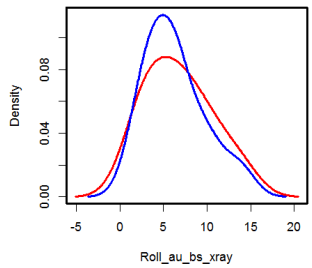
| | | | | |
|---|---|---|---|---|
| **AU** |  |  |  |  |
| **AG** |  |  |  |  |
| **AC** |  |  |  |  |
| **UA** |  |  |  |  |

Continue…

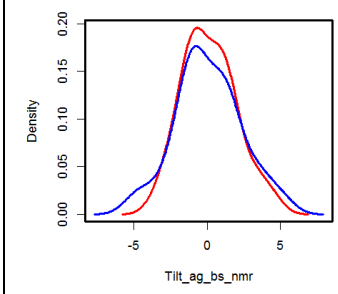
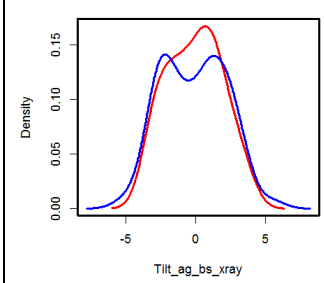
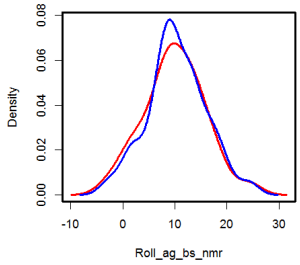
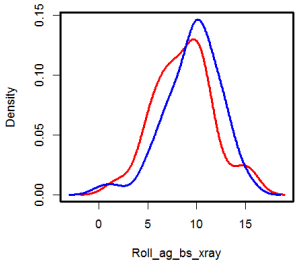
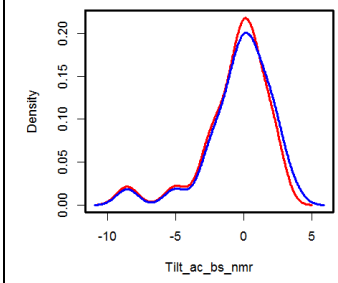
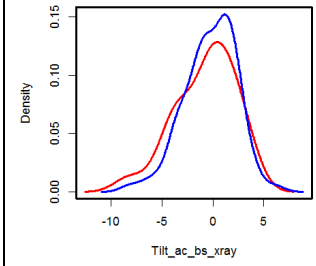
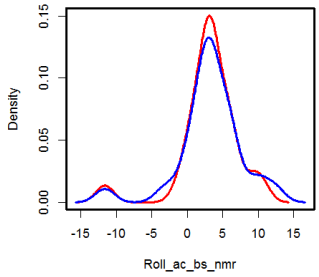
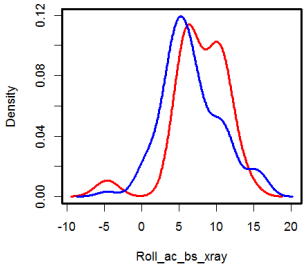
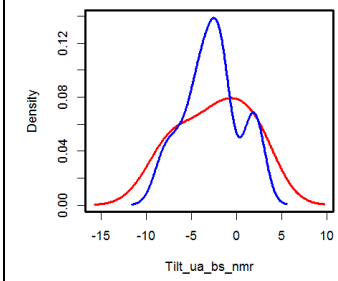
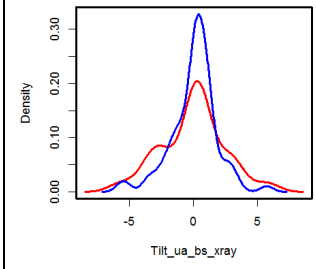
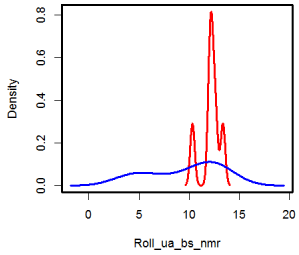
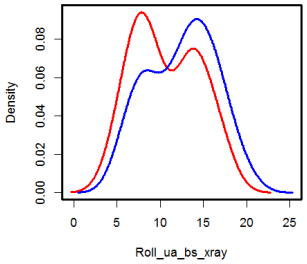
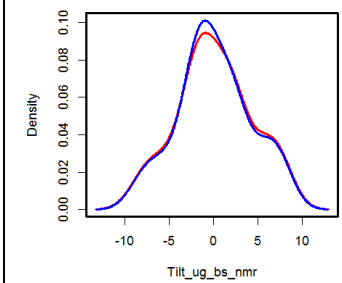
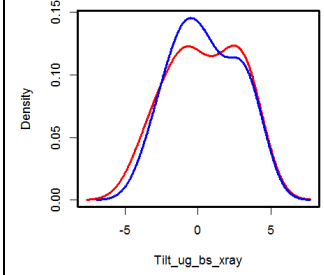
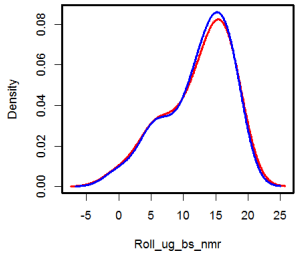
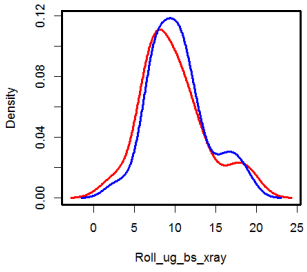
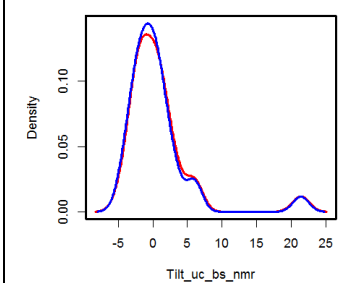
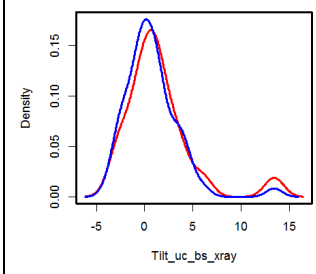
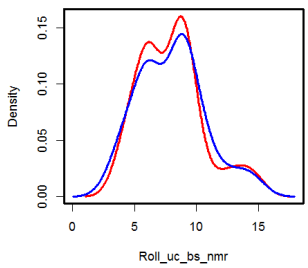
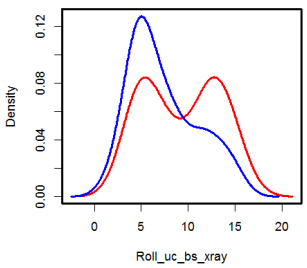
| | | | | |
|---|---|---|---|---|
| **UG** |  |  |  |  |
| **UC** |  |  |  |  |
| **GG** |  |  |  |  |
| **GC** |  |  |  |  |

Continue…

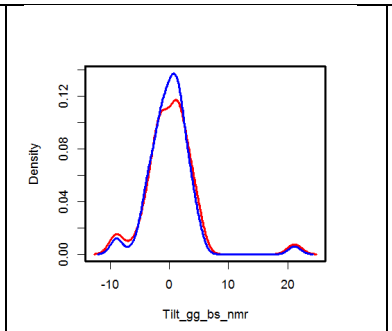
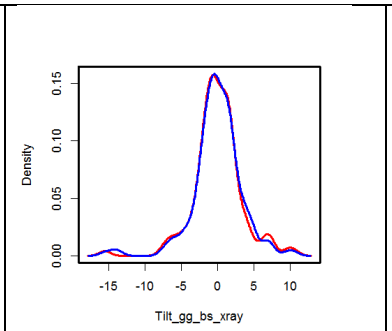
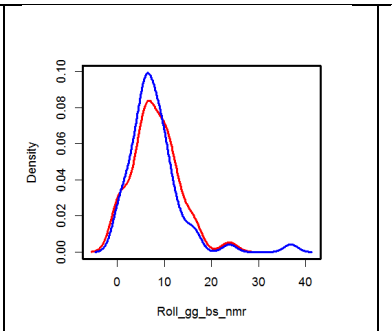
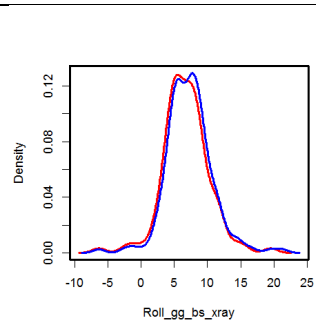
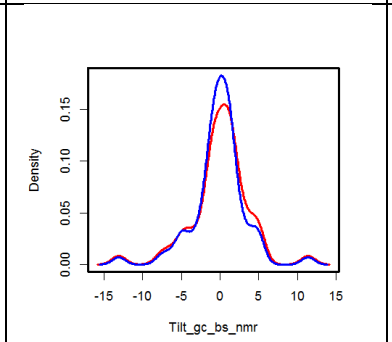
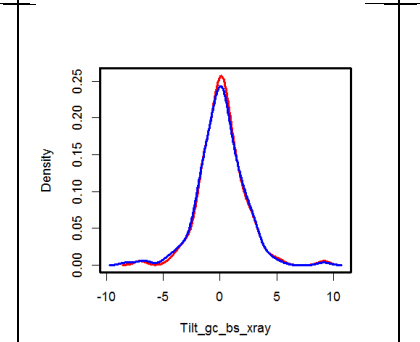
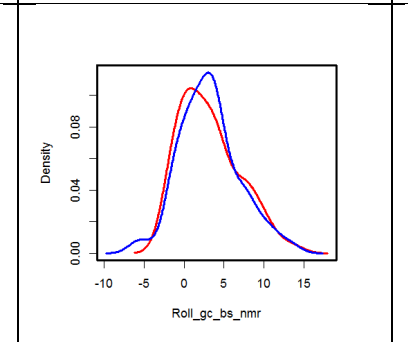
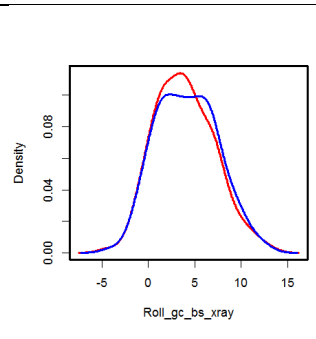
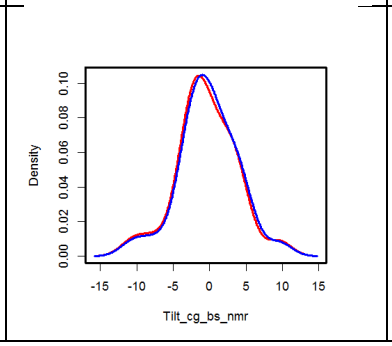
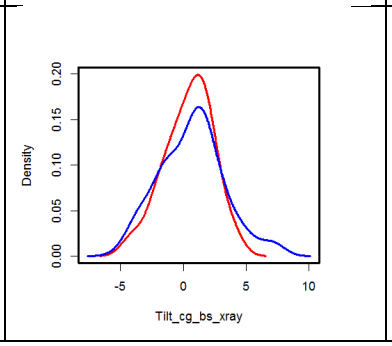
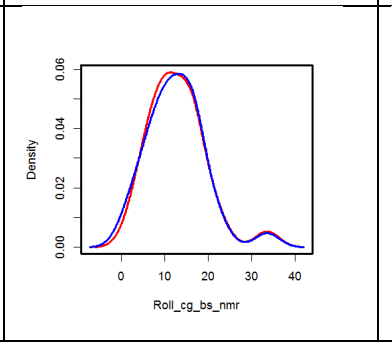
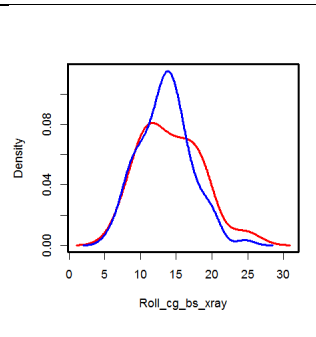
| | | | | |
|---|---|---|---|---|
| **CG** |  |  |  |  |

| Base pair step | **Tilt** | | **Roll** | |
|---|---|---|---|---|
| | **NMR** | **X-Ray** | **NMR** | **X-Ray** |
| **AA** |  |  |  |  |
| **AU** |  |  |  |  |

Continue…

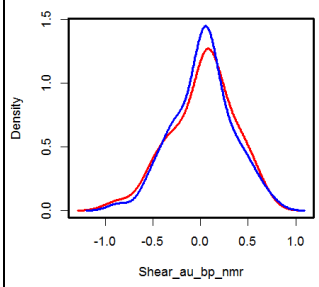
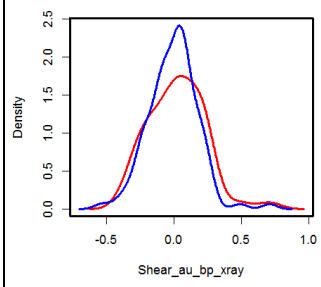
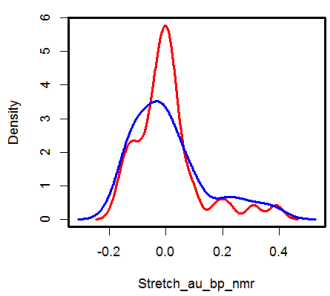
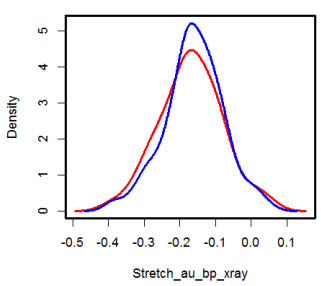
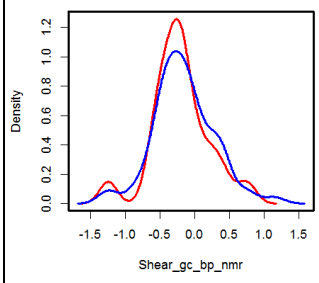
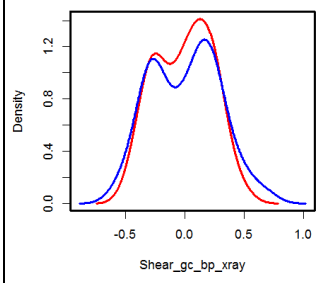
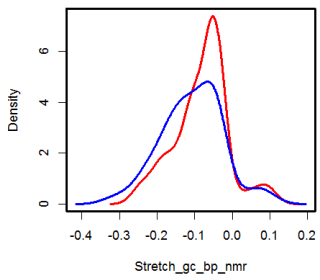
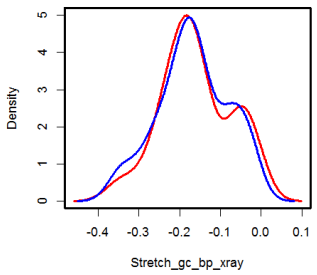
| | | | | |
|---|---|---|---|---|
| **AG** |  |  |  |  |
| **AC** |  |  |  |  |
| **UA** |  |  |  |  |
| **UG** |  |  |  |  |
| **UC** |  |  |  |  |

Continue…

| | | | | |
|---|---|---|---|---|
| **GG** |  |  |  |  |
| **GC** |  |  |  |  |
| **CG** |  |  |  |  |

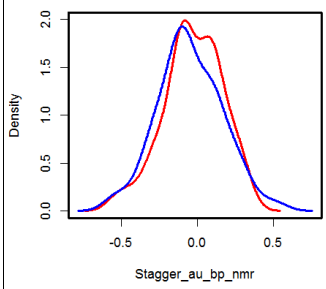
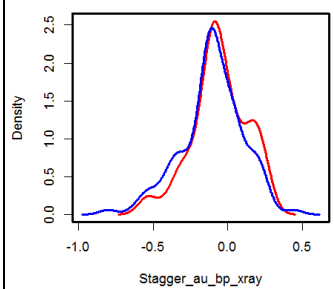
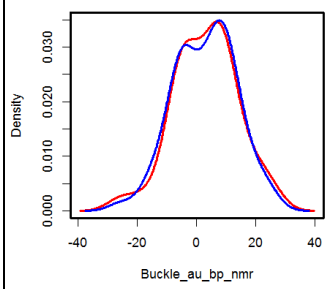
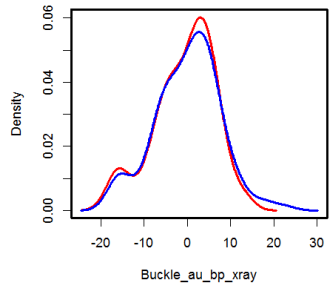
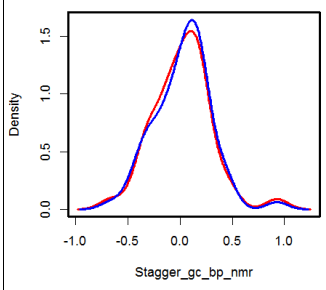
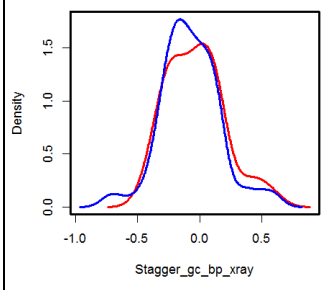
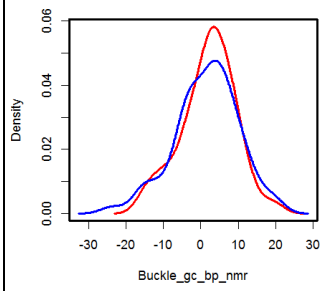
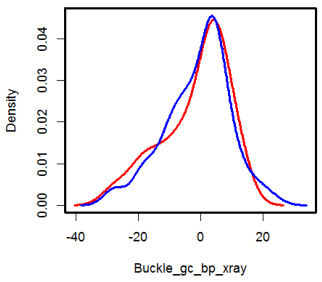
Continue…

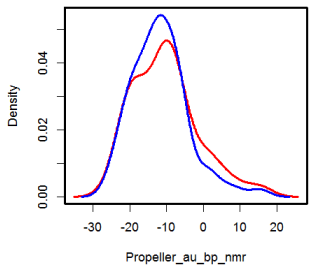
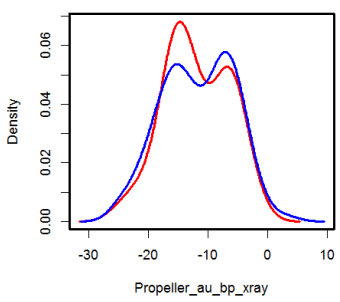
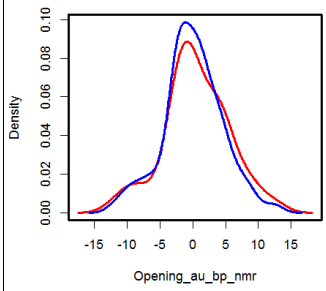
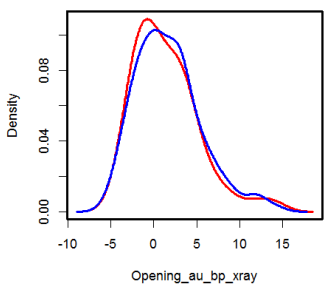
**Table 1(C). Density plots for all base pair and base pair step parameters of RNA-DNA duplexes**

| Base pair | Shear | | Stretch | |
|---|---|---|---|---|
| | **NMR** | **X-Ray** | **NMR** | **X-Ray** |
| **A-U** |  |  |  |  |
| **G-C** |  |  |  |  |

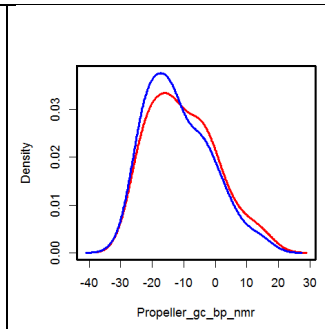
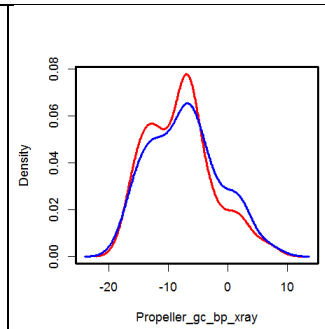
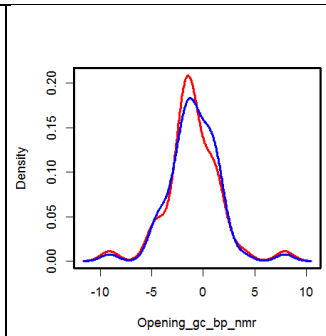
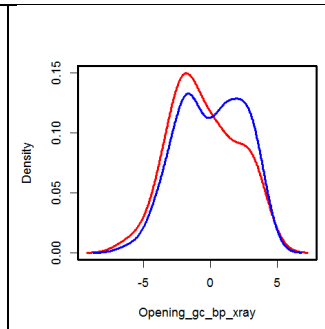
| Base pair | Stagger | | Buckle | |
|---|---|---|---|---|
| | **NMR** | **X-Ray** | **NMR** | **X-Ray** |

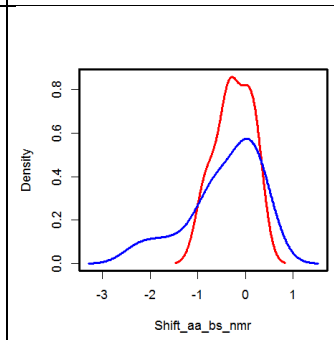
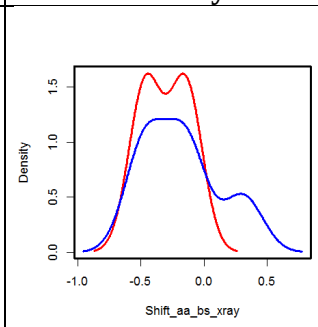
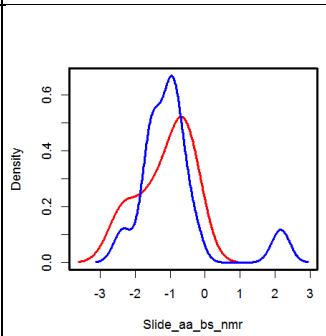
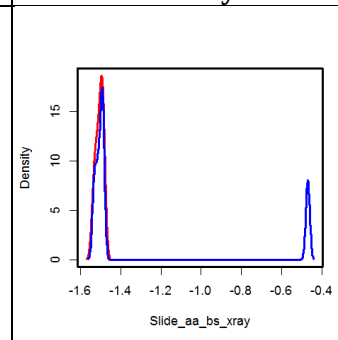
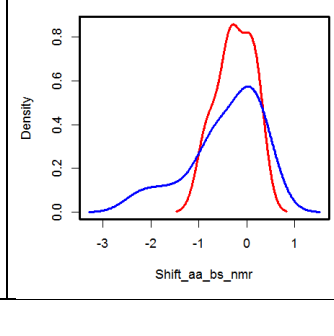
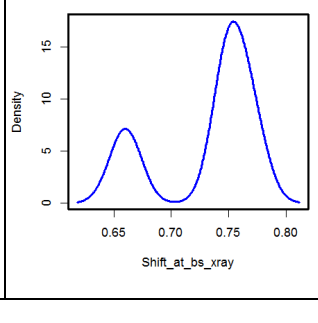
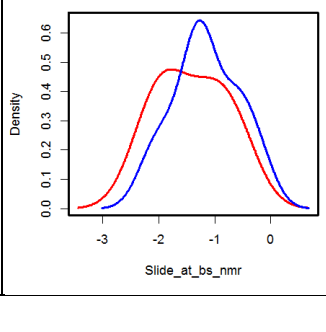
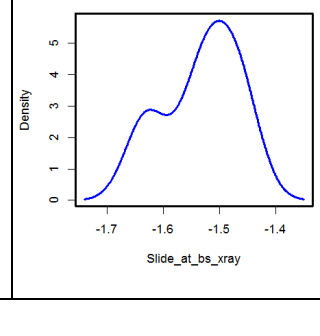
Continue…

| | | | | |
|---|---|---|---|---|
| **A-U** |  |  |  |  |
| **G-C** |  |  |  |  |

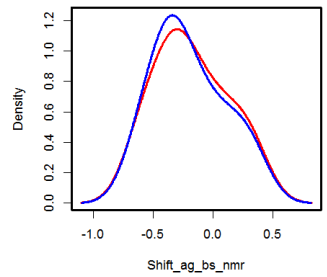
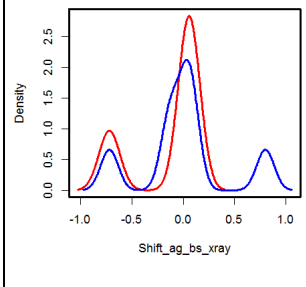
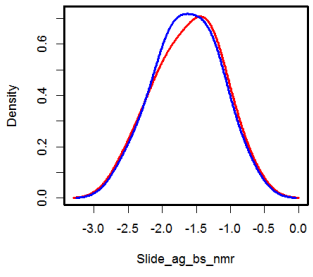
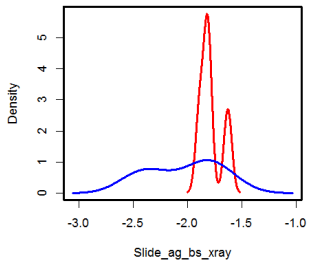
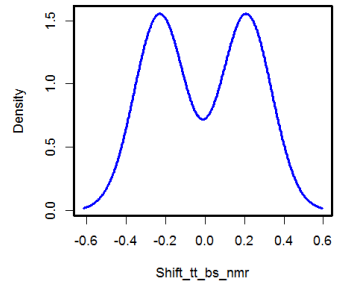
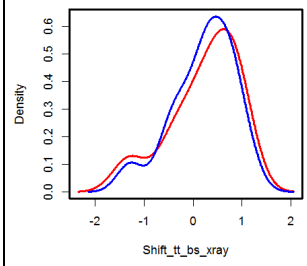
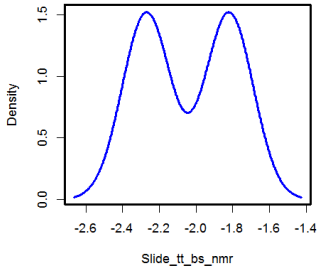
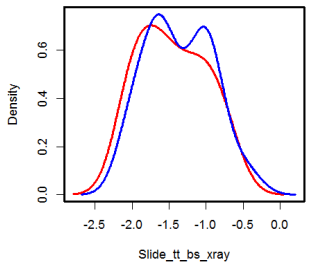
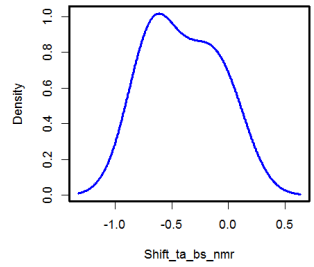
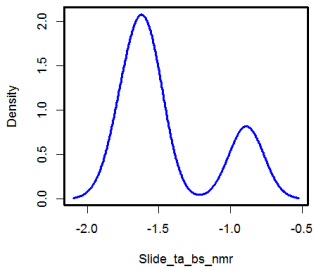
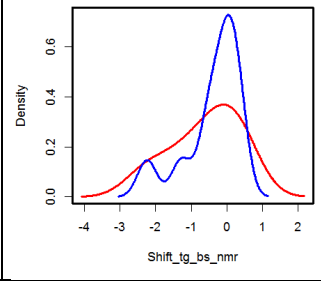
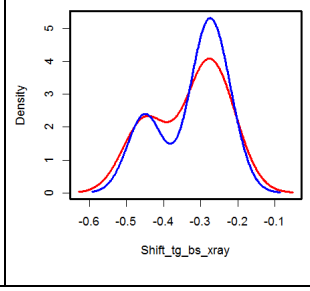
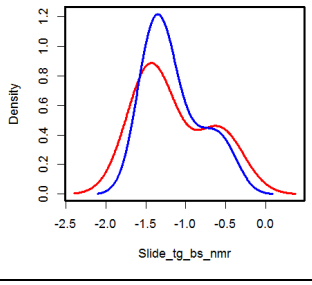
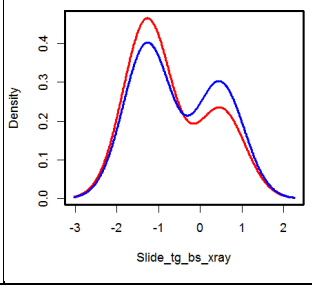
| Base pair | **Propeller** | | **Opening** | |
|---|---|---|---|---|
| | **NMR** | **X-Ray** | **NMR** | **X-Ray** |
| **A-U** |  |  |  |  |

Continue…

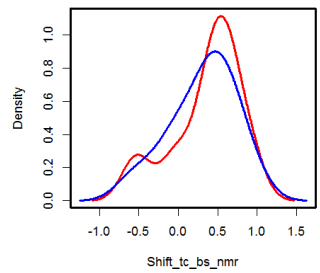
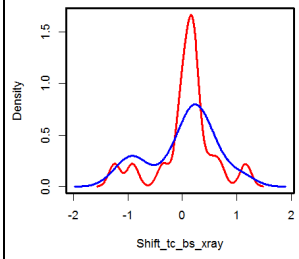
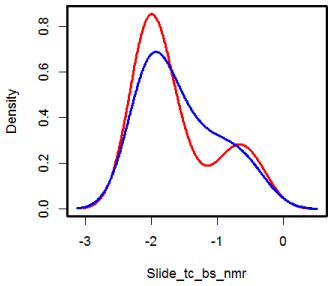
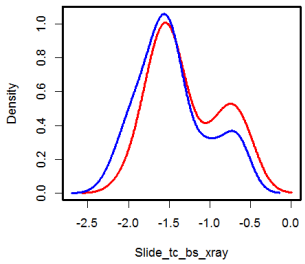
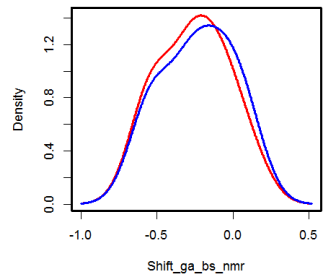
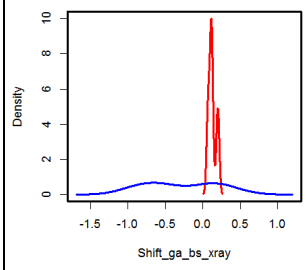
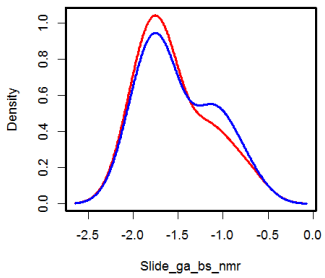
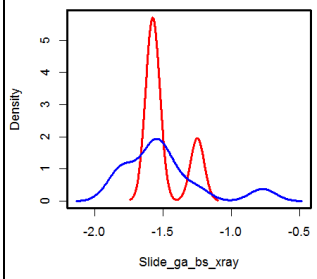
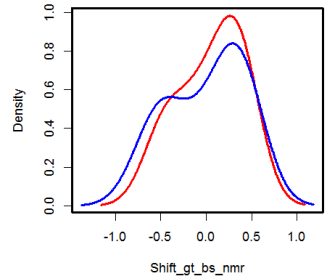
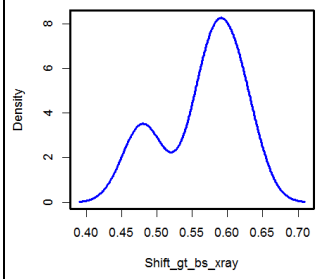
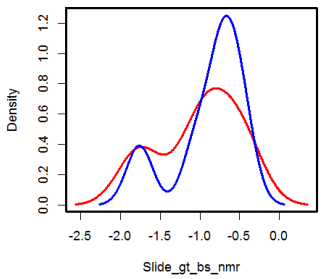
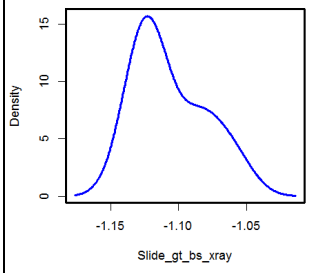
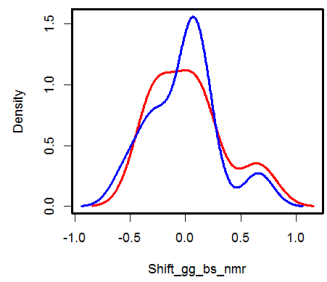
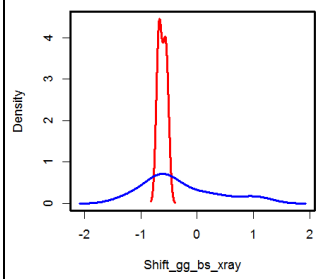
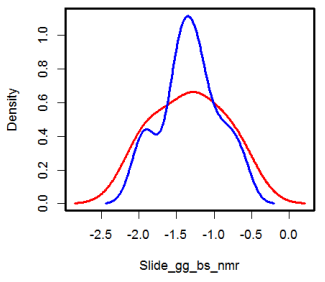
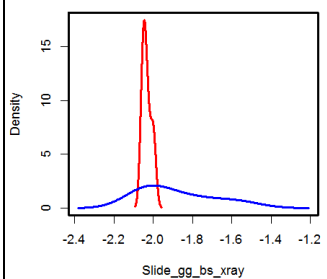
| | | | | |
|---|---|---|---|---|
| **G-C** |  |  |  |  |

| Base pair step | **Shift** | | **Slide** | |
|---|---|---|---|---|
| | **NMR** | **X-Ray** | **NMR** | **X-Ray** |
| **AA** |  |  |  |  |
| **AT** |  |  |  |  |

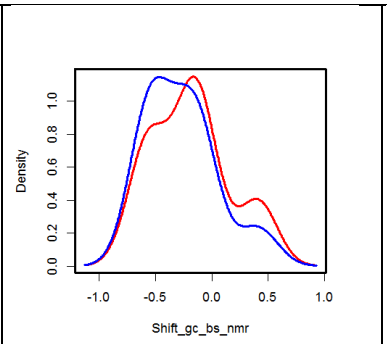
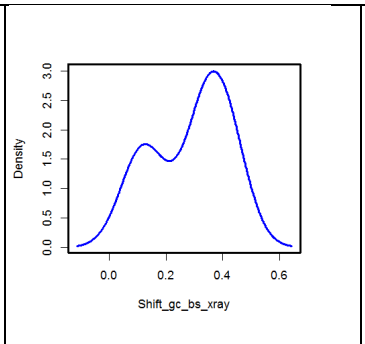
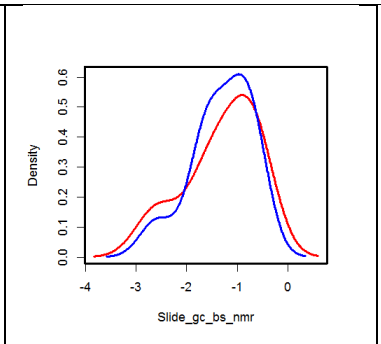
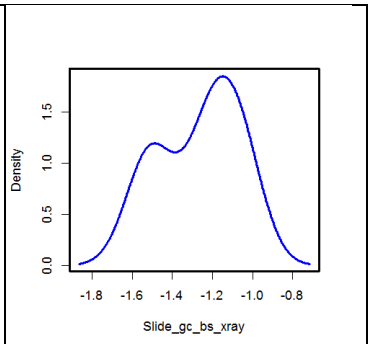
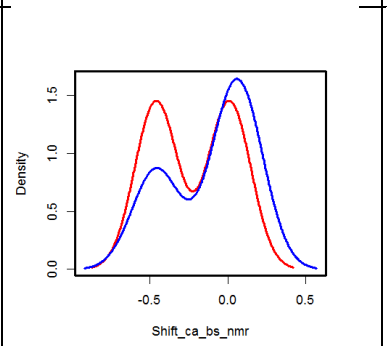
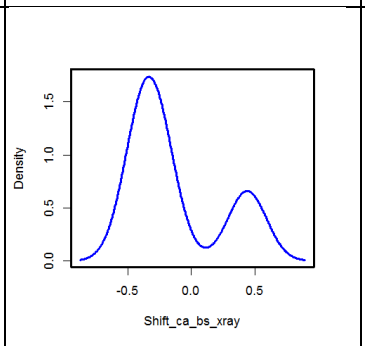
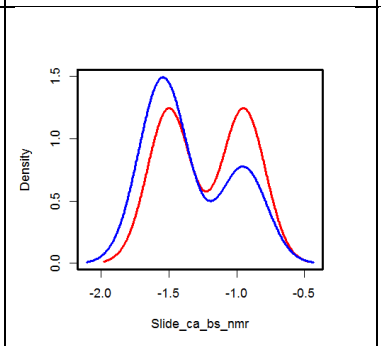
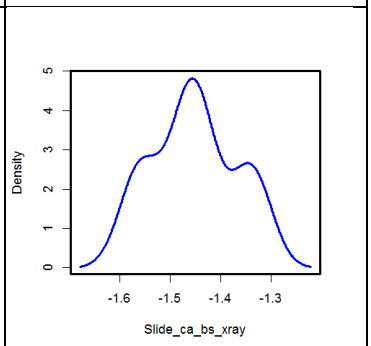
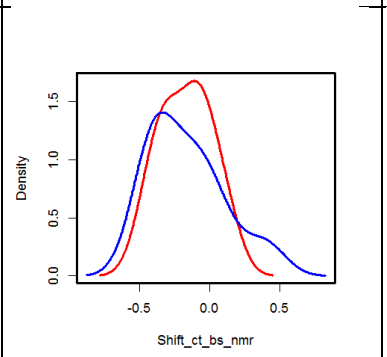
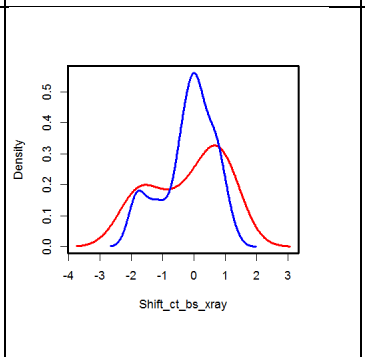
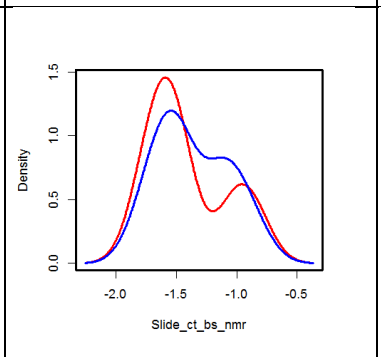
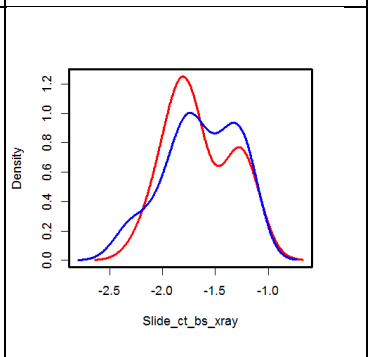
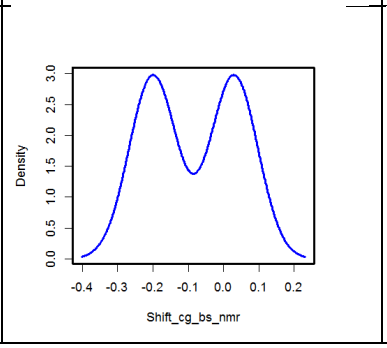
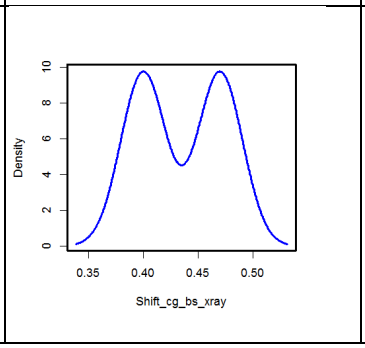
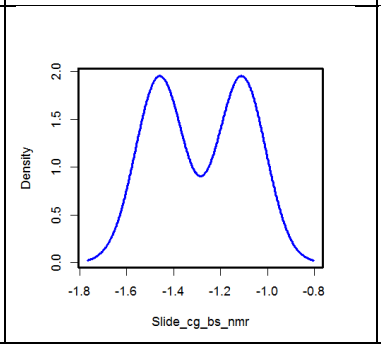
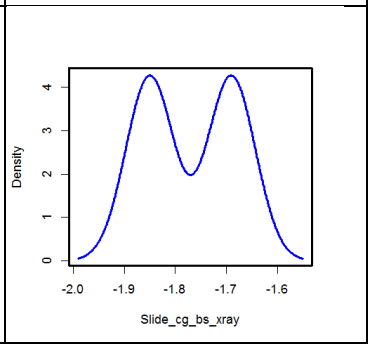
Continue…

| | | | | |
|---|---|---|---|---|
| **AG** |  |  |  |  |
| **TT** |  |  |  |  |
| **TA** |  | |  | |
| **TG** |  |  |  |  |

Continue…

| | | | | |
|---|---|---|---|---|
| **TC** |  |  |  |  |
| **GA** |  |  |  |  |
| **GT** |  |  |  |  |
| **GG** |  |  |  |  |

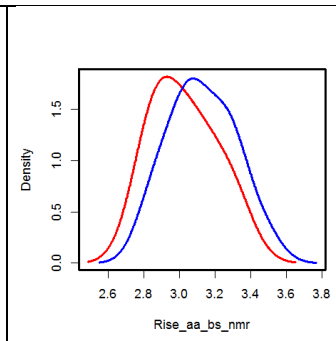
Continue…

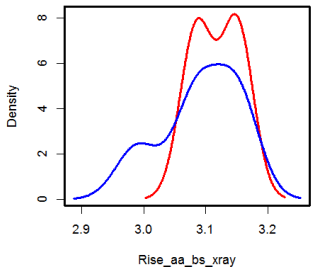
| | | | | |
|---|---|---|---|---|
| **GC** |  |  |  |  |
| **CA** |  |  |  |  |
| **CT** |  |  |  |  |
| **CG** |  |  |  |  |

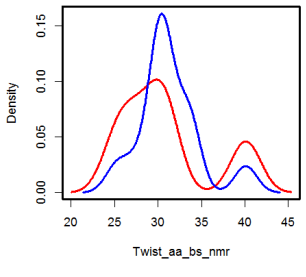
| Base pair step | **Rise** | | **Twist** | |
|---|---|---|---|---|
| | **NMR** | **X-Ray** | **NMR** | **X-Ray** |

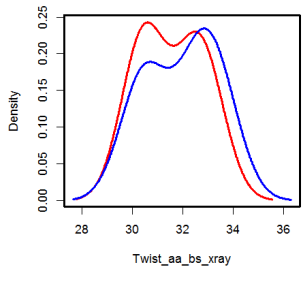
Continue…

**AA**

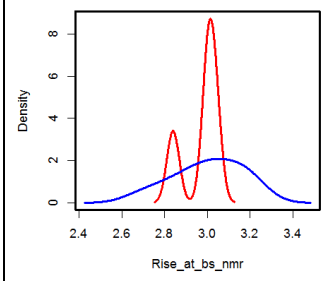


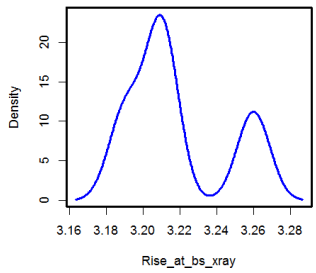



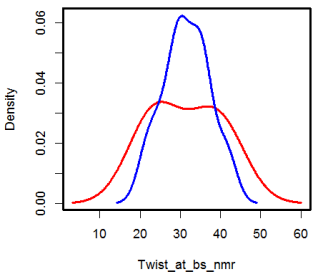



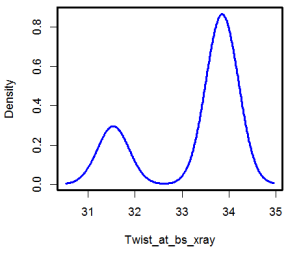




**AT**

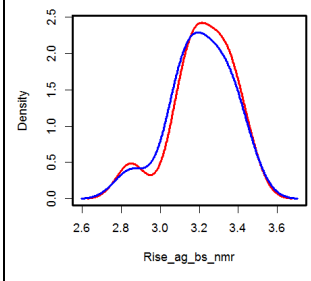


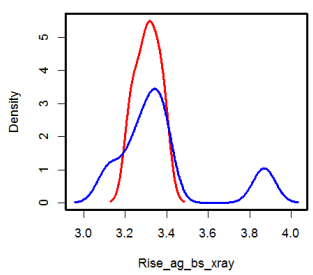



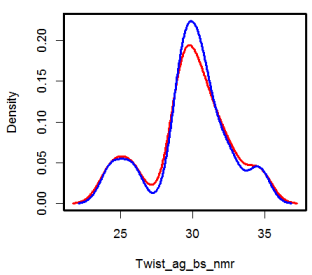



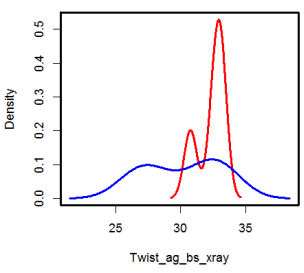




**AG**

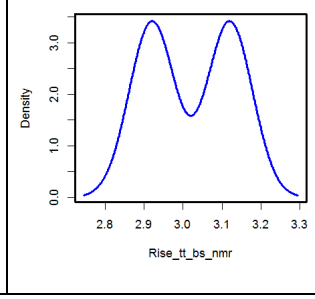


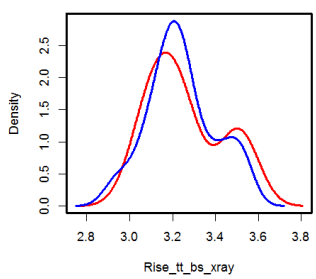



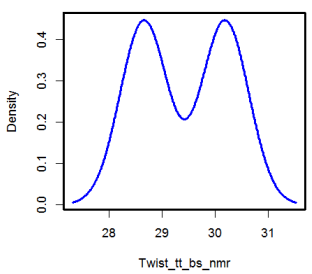



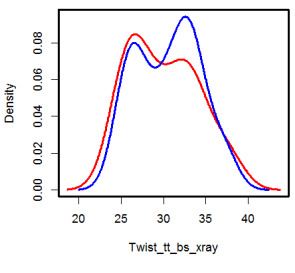




**TT**

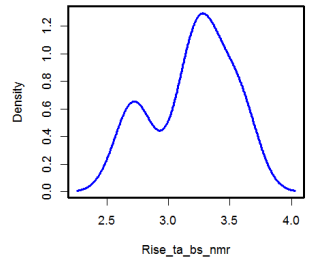
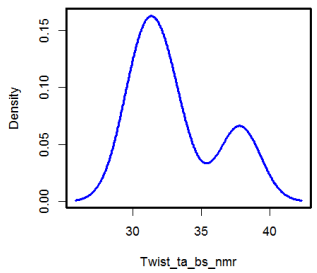
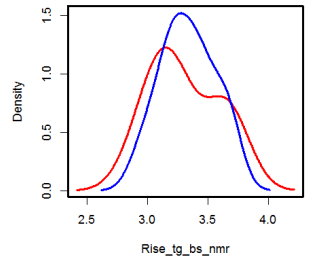
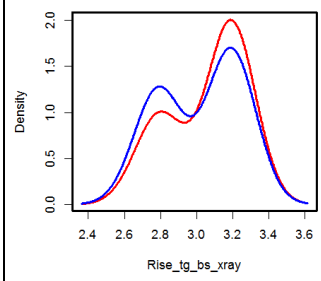
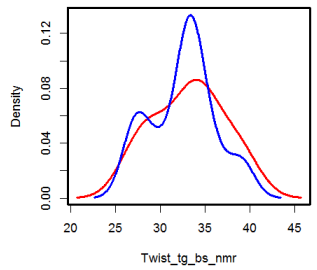
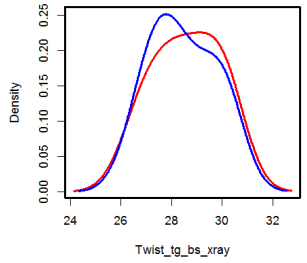
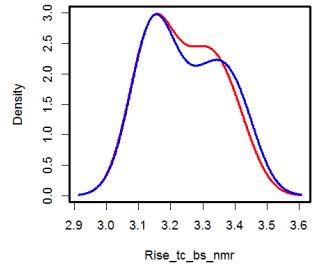
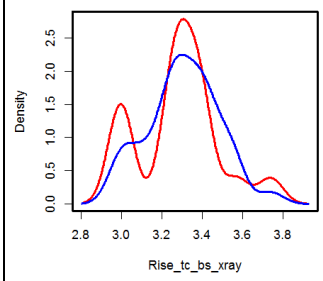
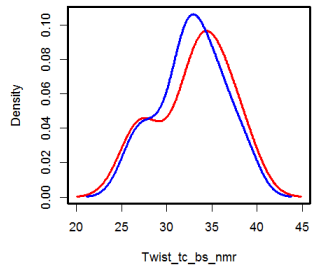
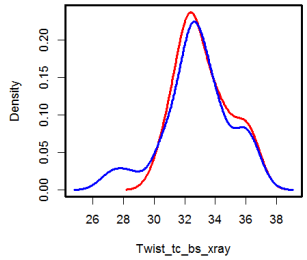
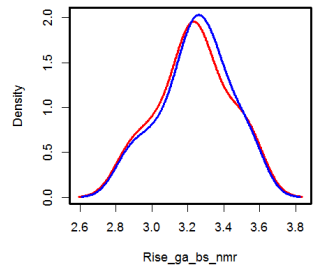
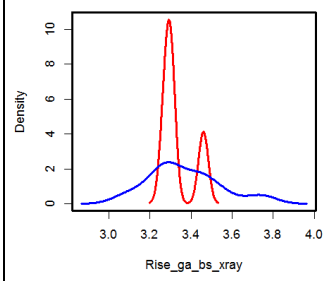
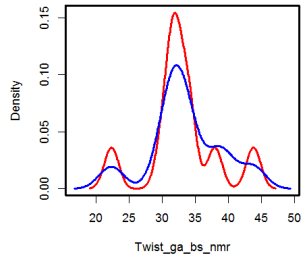
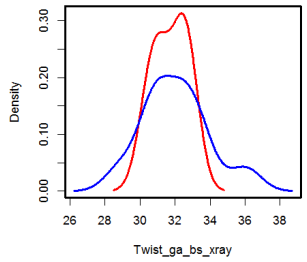
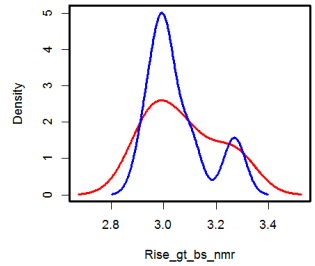
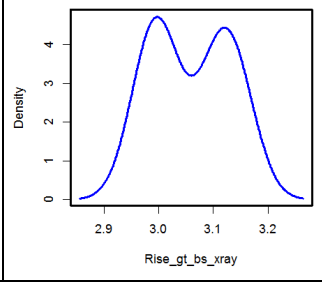
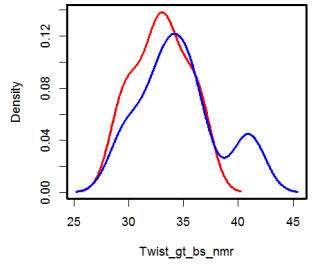
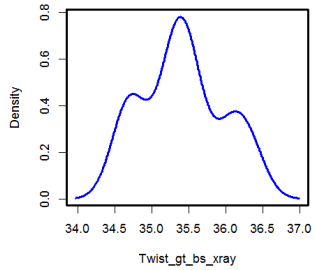


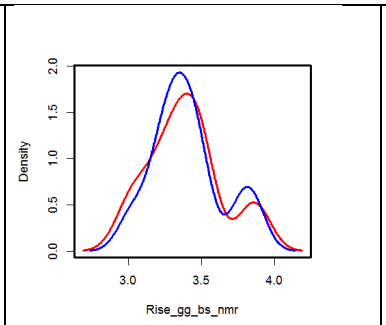
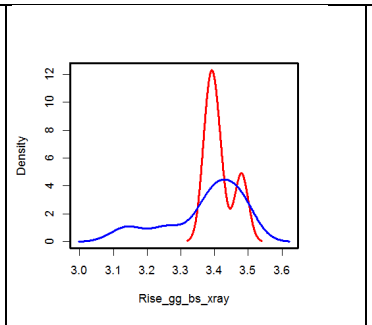
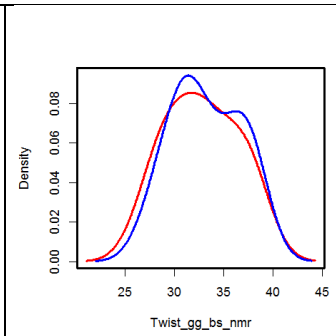
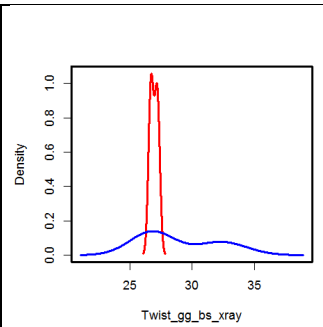
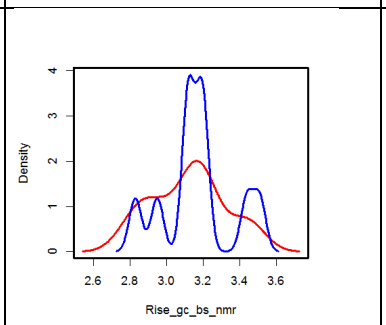
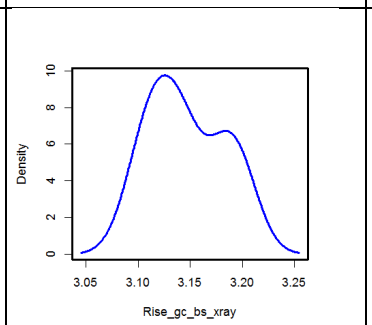
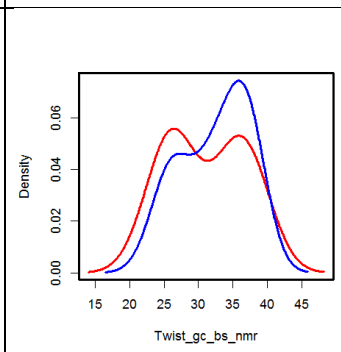
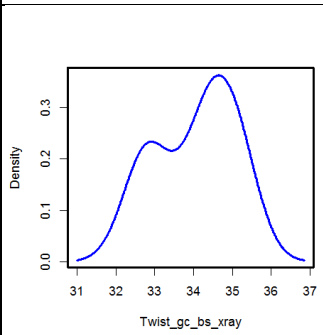
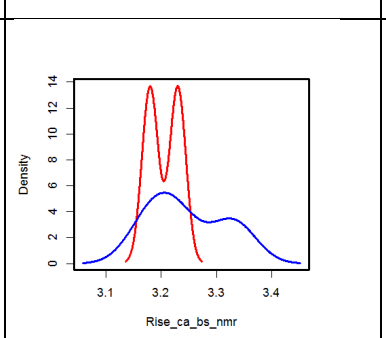
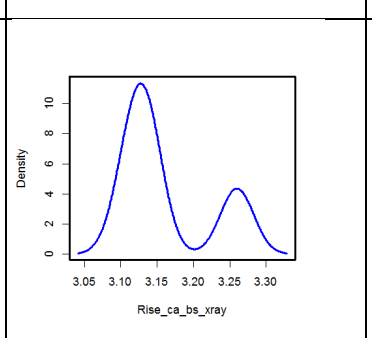
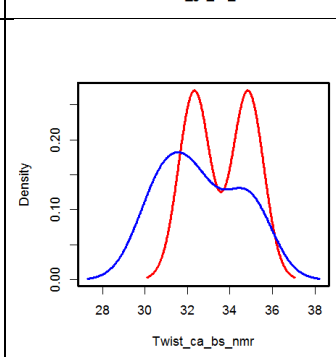
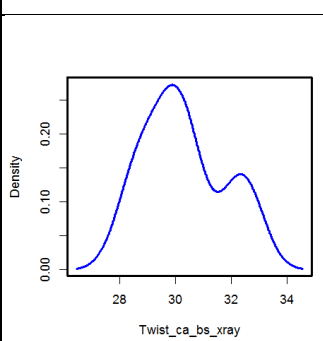
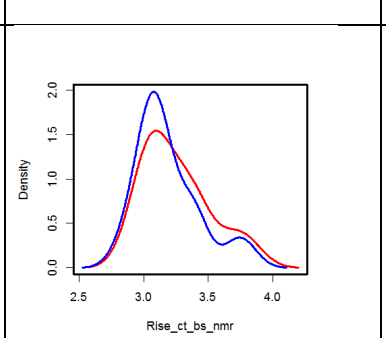
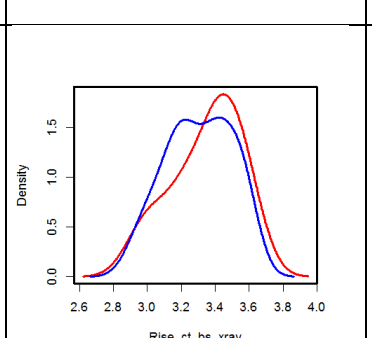
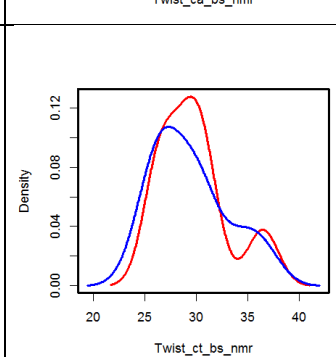
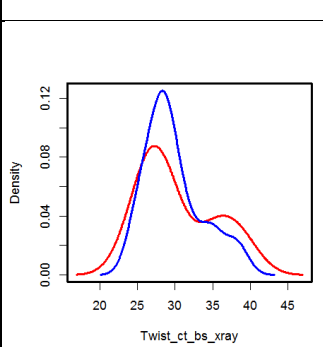



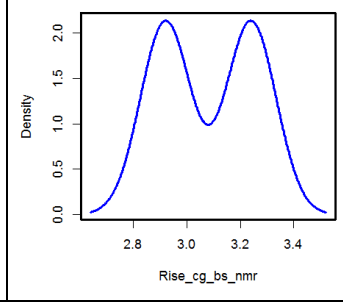
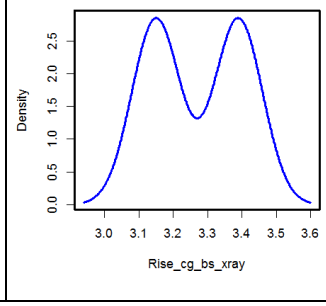
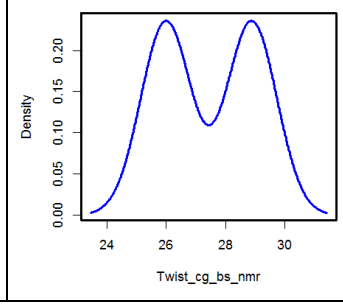
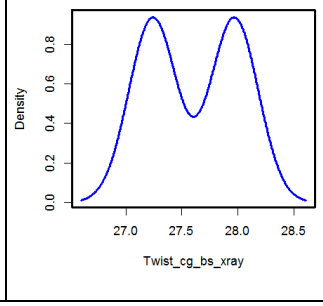

Continue…

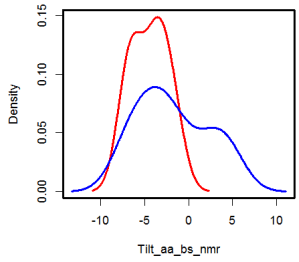
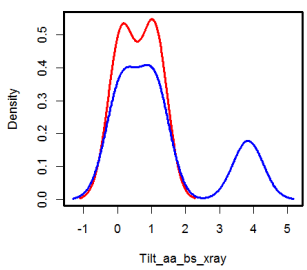
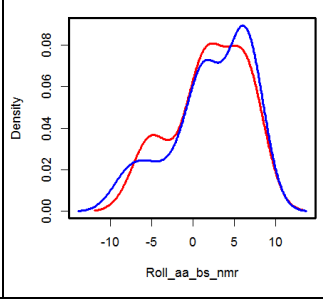
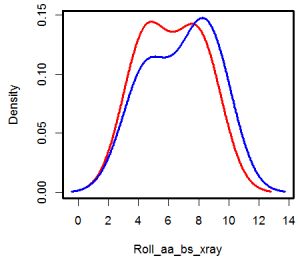
| | | | | |
|---|---|---|---|---|
| **TA** |  | |  | |
| **TG** |  |  |  |  |
| **TC** |  |  |  |  |
| **GA** |  |  |  |  |
| **GT** |  |  |  |  |

Continue…

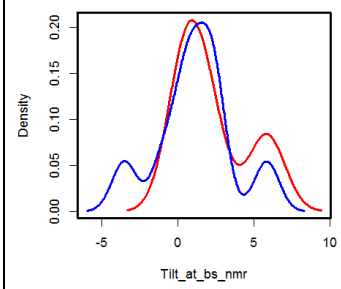
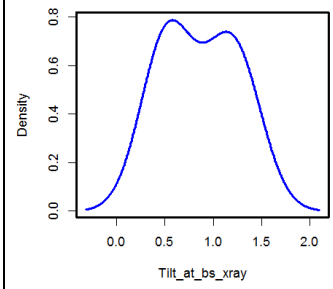
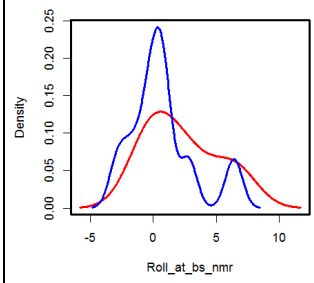
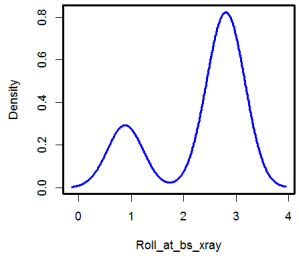
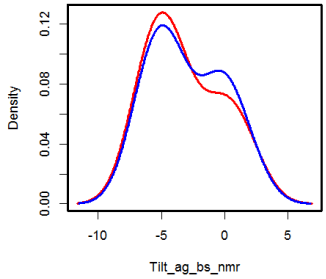
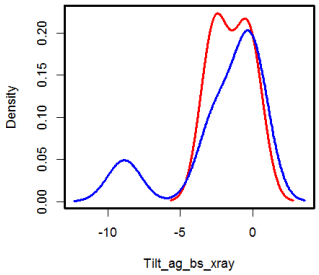
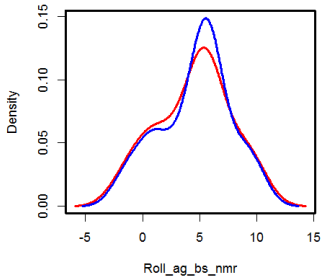
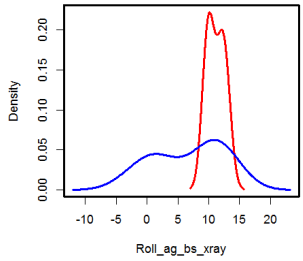
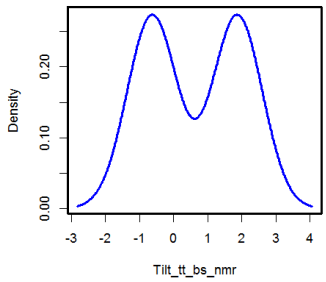
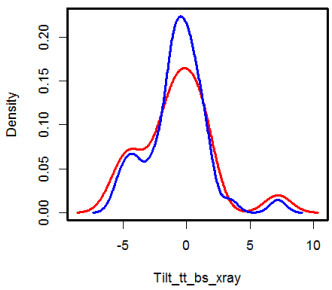
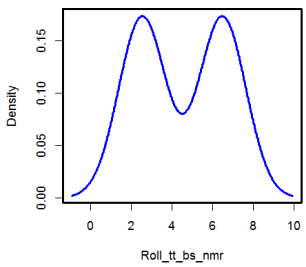
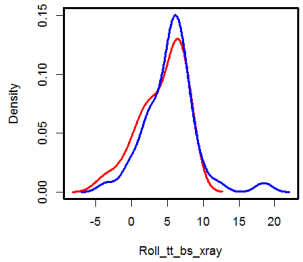
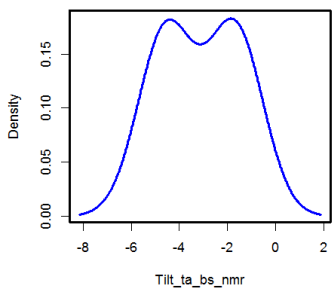
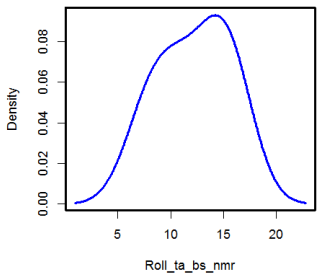
| | | | | |
|---|---|---|---|---|
| **GG** |  |  |  |  |
| **GC** |  |  |  |  |
| **CA** |  |  |  |  |
| **CT** |  |  |  |  |

Continue…

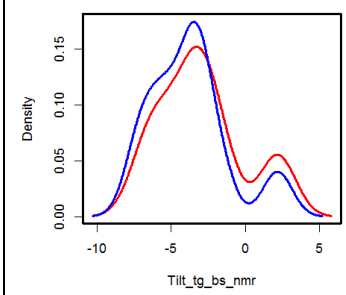
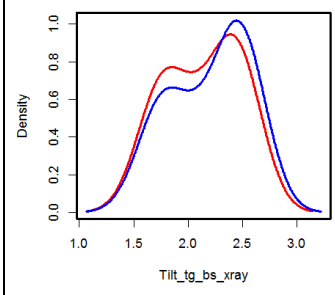
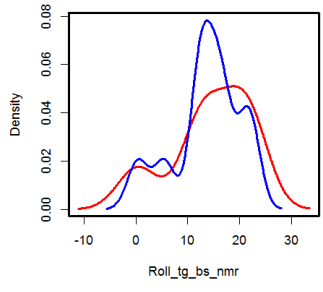
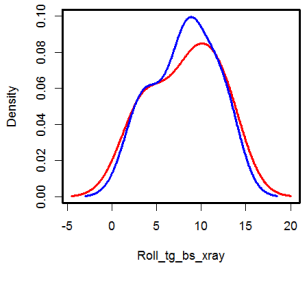
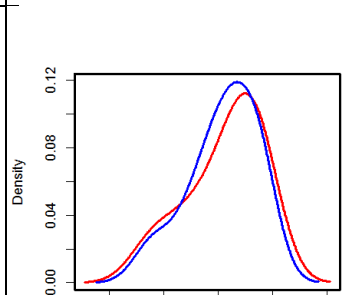
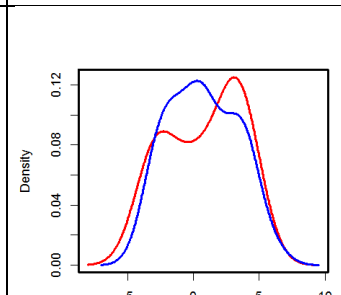
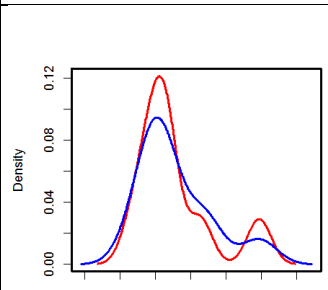
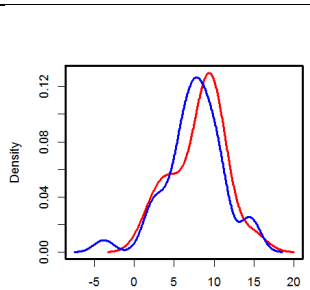
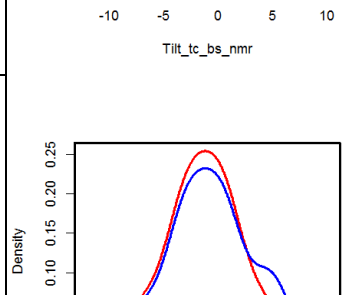
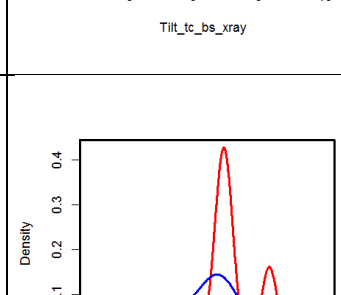
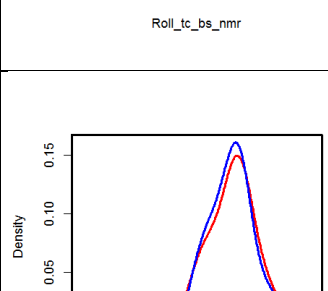
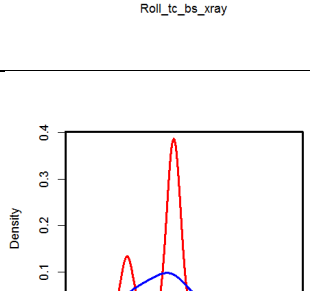
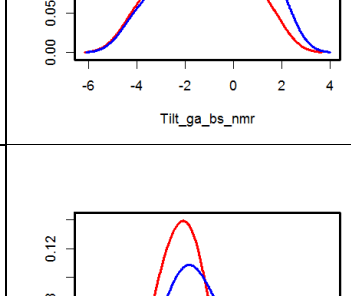
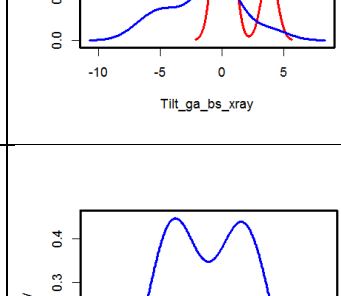
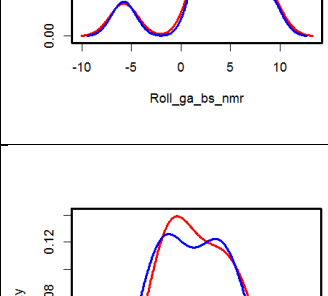
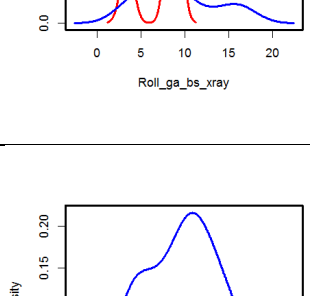
| | | | | |
|---|---|---|---|---|
| **CG** |  |  |  |  |

| Base pair step | **Tilt** | | **Roll** | |
|---|---|---|---|---|
| | **NMR** | **X-Ray** | **NMR** | **X-Ray** |
| **AA** |  |  |  |  |

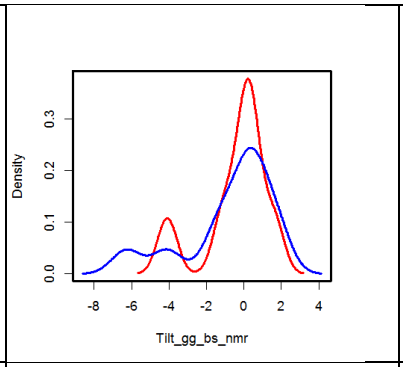
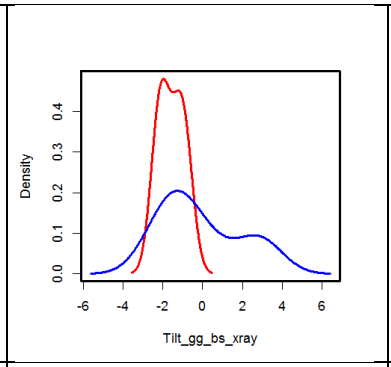
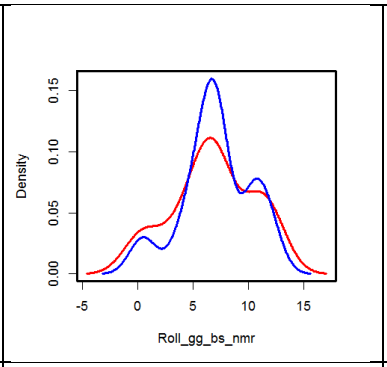
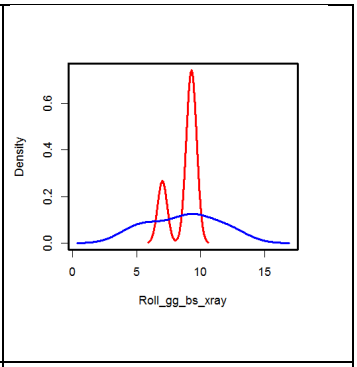
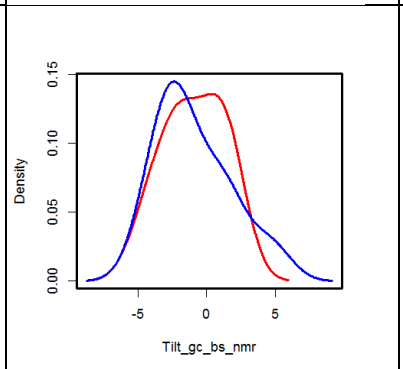
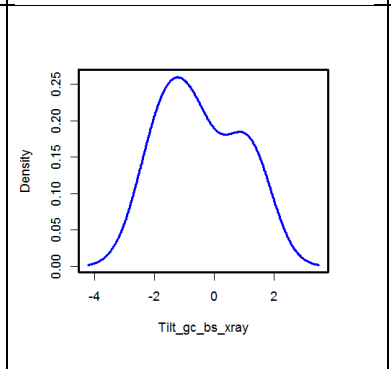
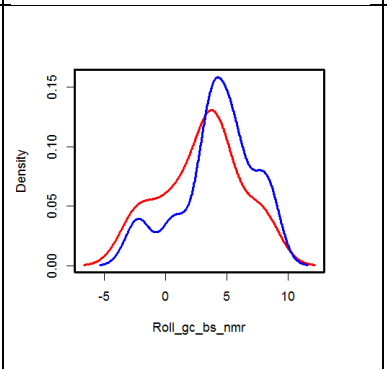
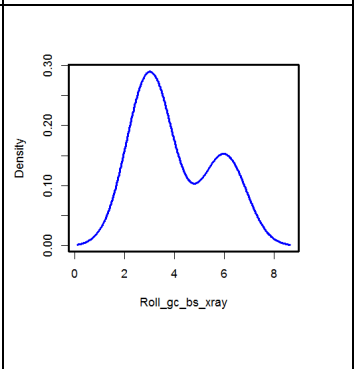
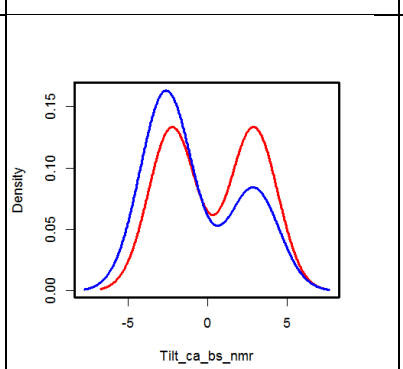
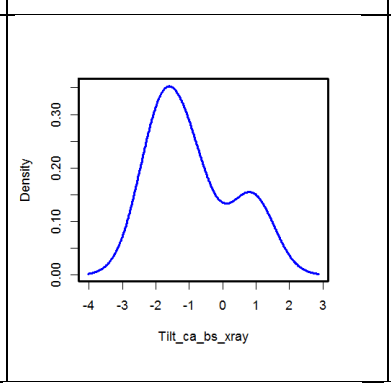
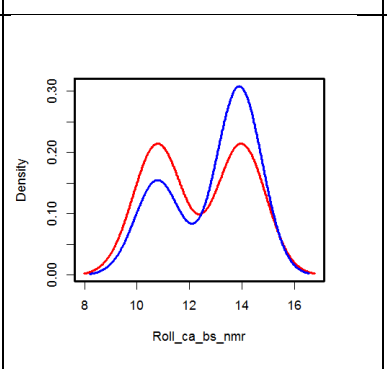
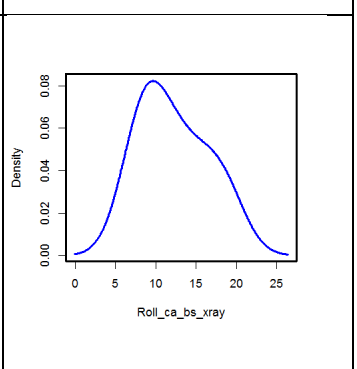
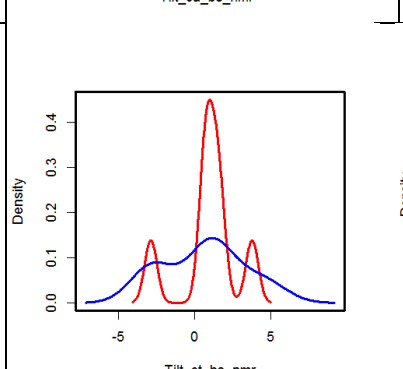
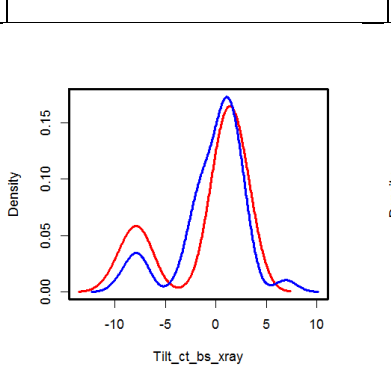
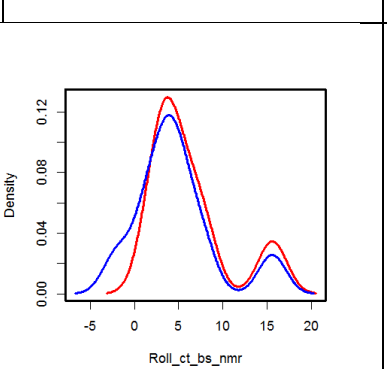
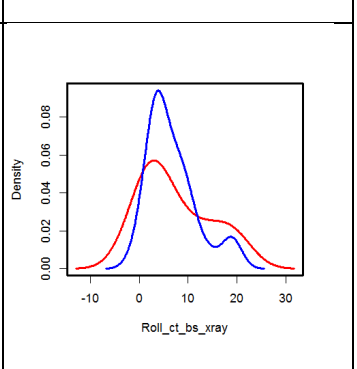
Continue…

| | | | | |
|---|---|---|---|---|
| **AT** |  |  |  |  |
| **AG** |  |  |  |  |
| **TT** |  |  |  |  |
| **TA** |  | |  | |

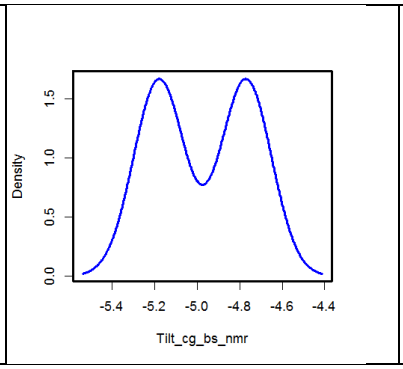
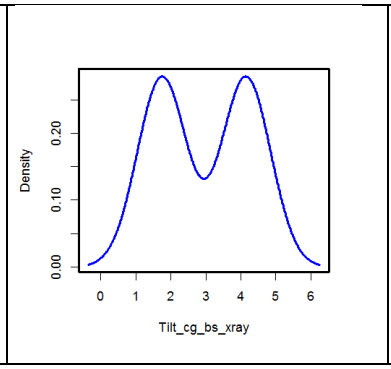
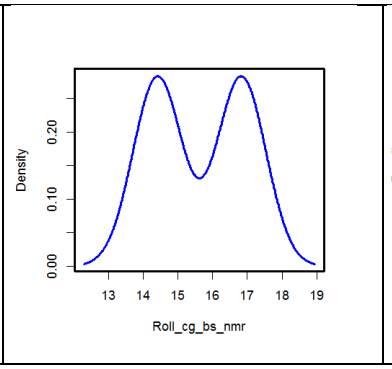
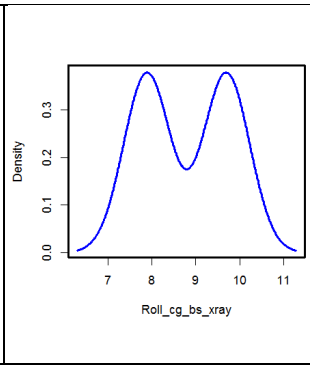
Continue…

| | | | | |
|---|---|---|---|---|
| **TG** |  |  |  |  |
| **TC** |  |  |  |  |
| **GA** |  |  |  |  |
| **GT** |  |  |  |  |

Continue…

| | | | | |
|---|---|---|---|---|
| **GG** |  |  |  |  |
| **GC** |  |  |  |  |
| **CA** |  |  |  |  |
| **CT** |  |  |  |  |

Continue…

| | | | | |
|---|---|---|---|---|
| **CG** |  |  |  |  |

1. Olson, W.K., et al., *DNA sequence-dependent deformability deduced from protein-DNA crystal complexes.* Proc Natl Acad Sci U S A, 1998. **95**(19): p. 11163-8.

Continue…