Supporting Information

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Radial distribution functions (RDFs)

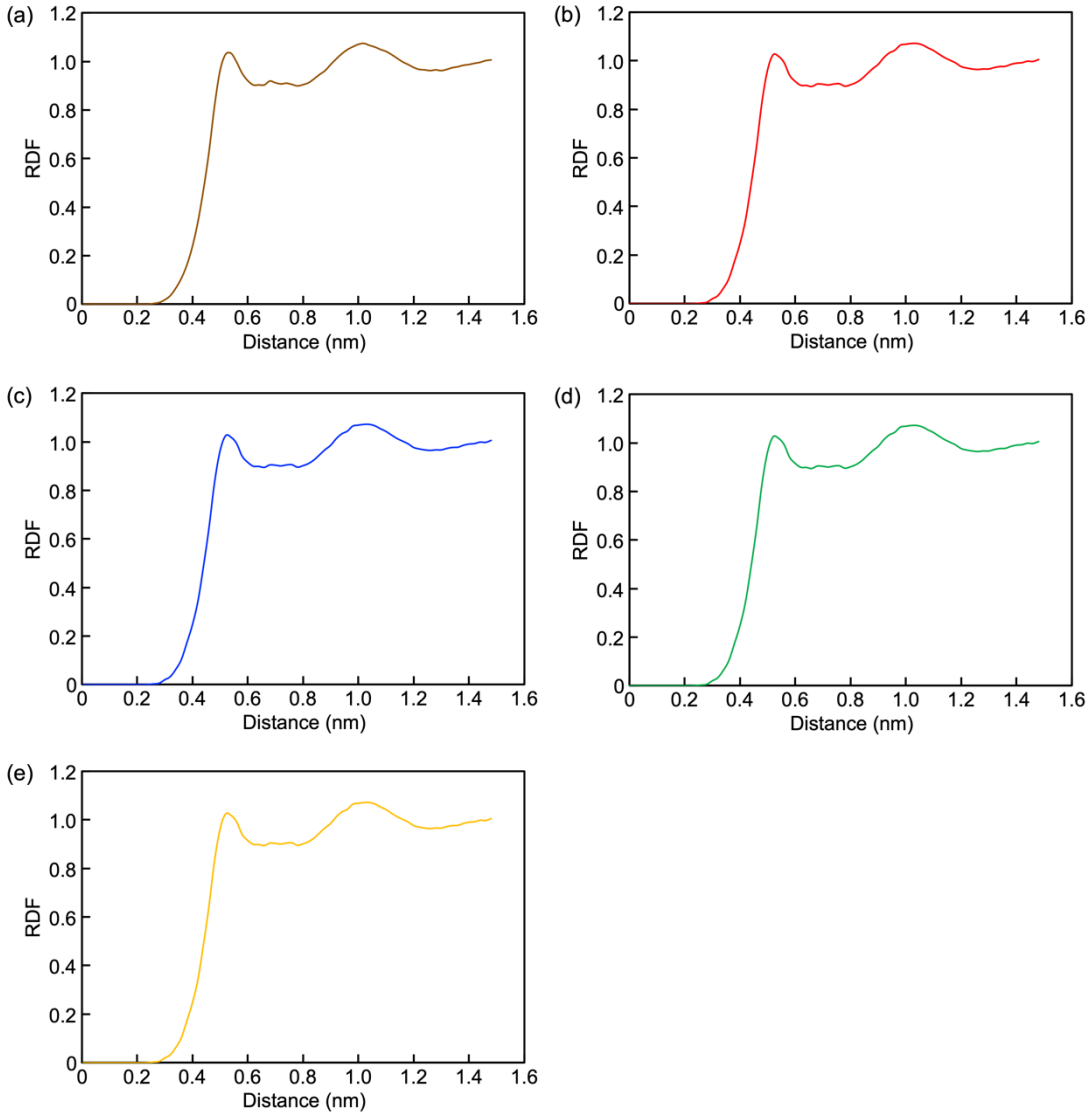

Figure S1. Radial distribution functions of the center of the mass of MBBA molecules for (a) pure MBBA, (b) **N-Ru-Br0**, (c) **N-Ru-Br1**, (d) **N-Ru-trop**, and **N-811**.

Intermolecular interaction energies

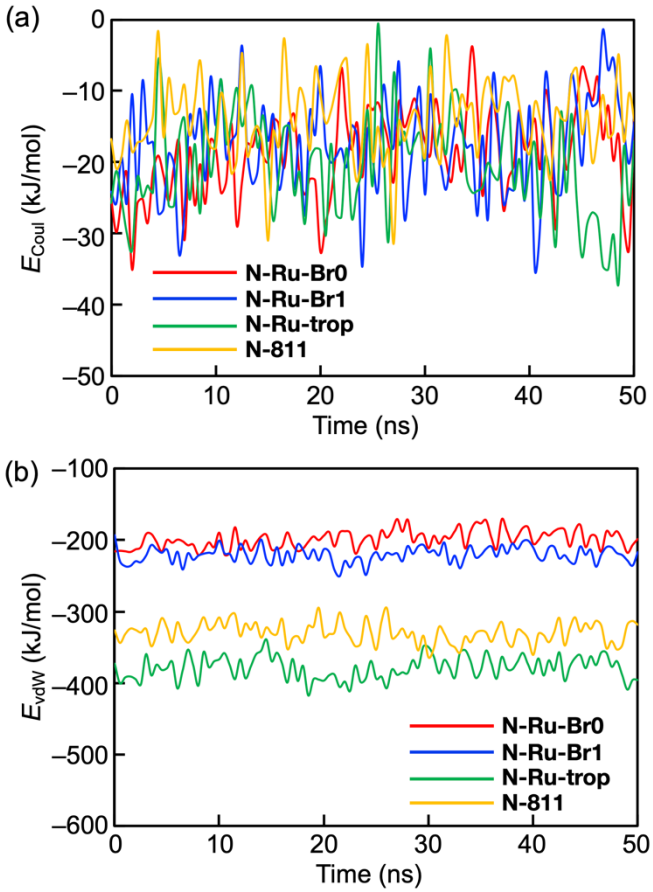

Figure S2. Time dependence of (a) Coulomb and (b) van der Waals interaction energies between the Δ-isomer of the chiral dopant molecule and MBBA molecules for **N-Ru-Br0**, **N-Ru-Br1**, **N-Ru-trop**, and **N-811** during the last 50 ns of equilibration runs.

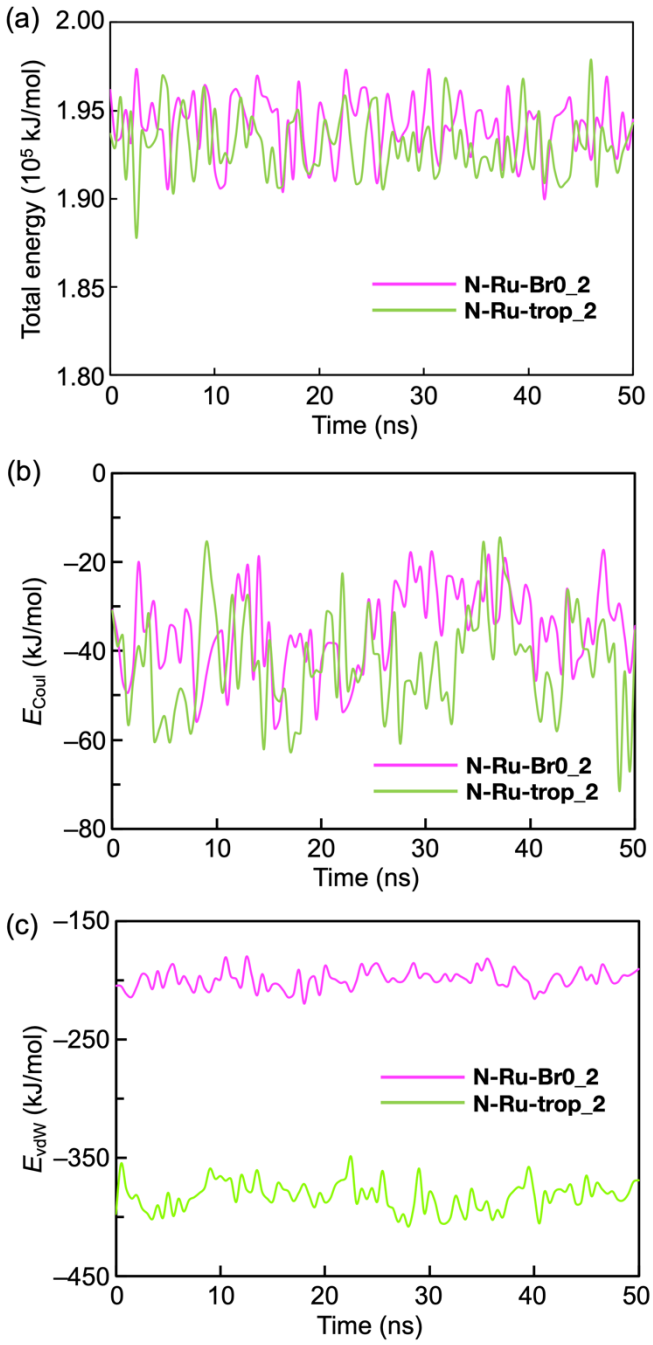

Figure S3. Time dependence of (a) total interaction energies and (b) Coulomb and (c) van der Waals interaction energies between the Δ-isomer of the chiral dopant molecule and MBBA molecules for **N-Ru-Br0_2** and **N-Ru-trop_2** during the last 50 ns of equilibration runs.

Order parameter

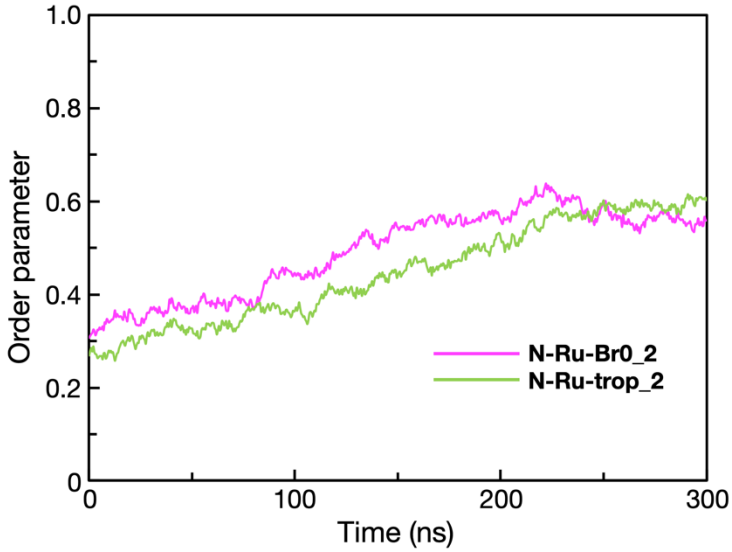

Figure S4. Time dependence of nematic order parameter for **N-Ru-Br0_2** and **N-Ru-trop_2.**

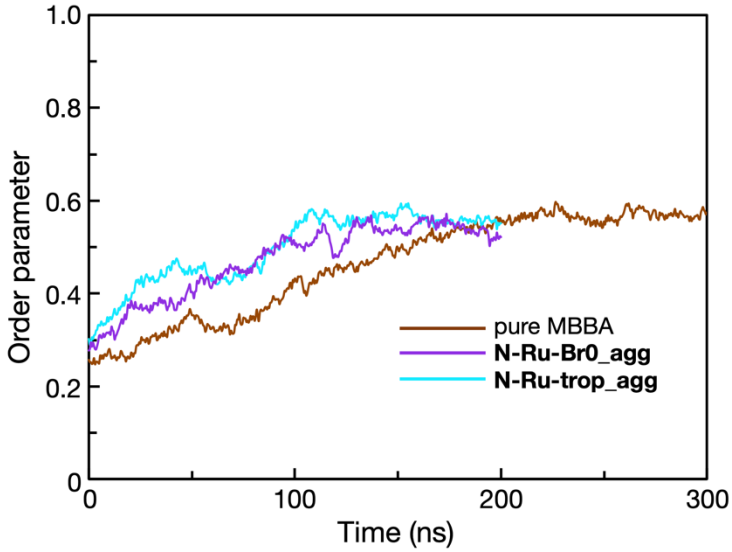

Figure S5. Time dependence of nematic order parameter for **N-Ru-Br0_agg** and **N-Ru-trop_agg** in which a pair of Δ- and Λ-isomers was restraint in the initial position.

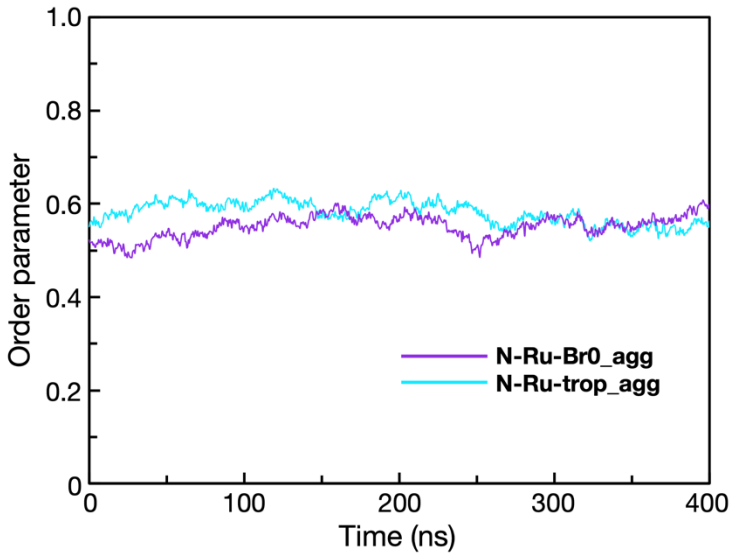

Figure S6. Time dependence of nematic order parameter for **N-Ru-Br0_agg** and **N-Ru-trop_agg** without any positional restraints.

Mean square displacements (MSDs)

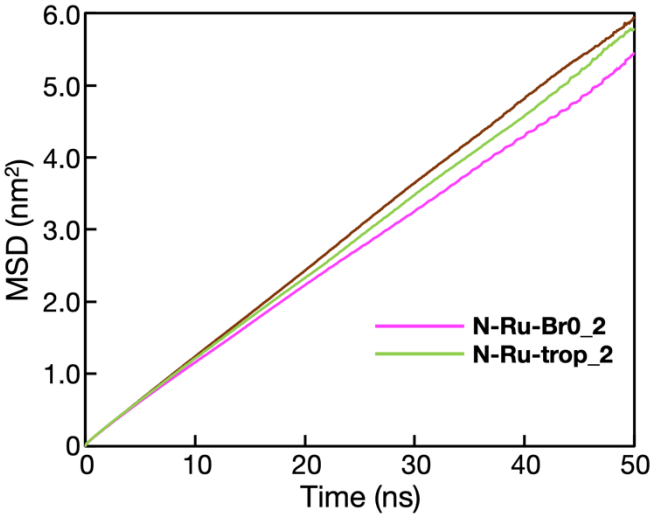

Figure S7. Mean square displacements of MBBA molecules during the last 50 ns of equilibration runs for **N-Ru-Br0_2** and **N-Ru-trop_2**.

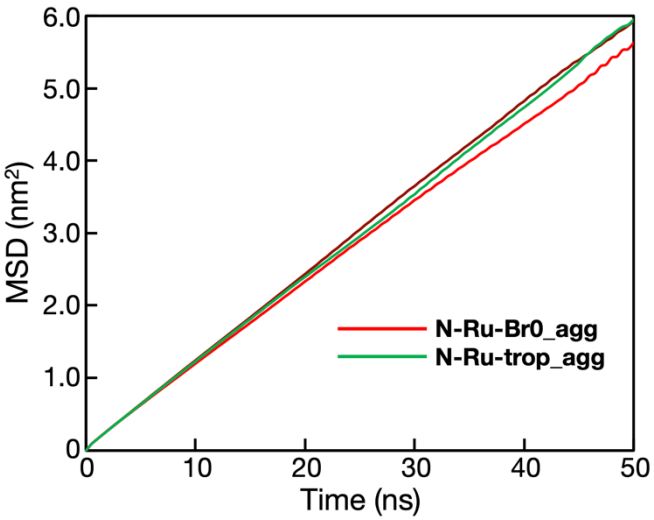

Figure S8. Mean square displacements of MBBA molecules during the last 50 ns of equilibration runs without any positional restraints for **N-Ru-Br0_agg** and **N-Ru-trop_agg**.

Distance between Δ- and Λ-isomers

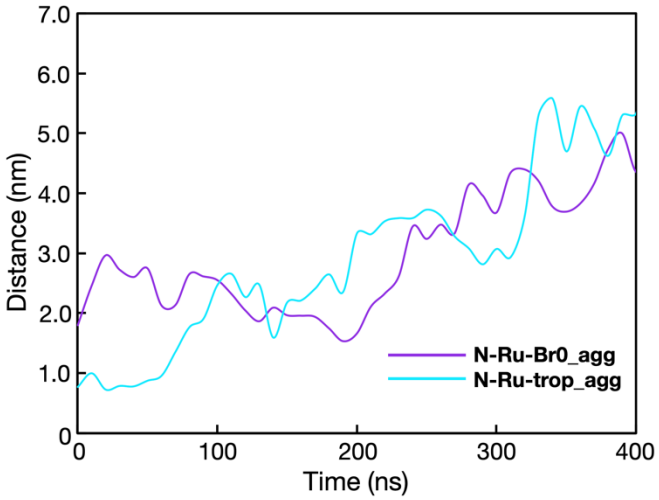

Figure S9. Time dependence of distances between Δ- and Λ-isomers during 400 ns equilibration runs without any positional restraints for **N-Ru-Br0_agg** and **N-Ru-trop_agg**.