Robotic-inspired approach to multi-domain membrane receptor conformation space: theory and SARS-CoV-2 spike protein case study

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Table 1: Points definition

Point	Definition
Base	Z coordinate of COM^a of P atoms of lower leaflet lipid molecules + XY coordinates of Joint 1
Joint 1	COM of C_α atoms of residues 1233-1237 of three chains A B C
Joint 2	COM of C_α atoms of residues 1207-1215 of three chains A B C
Joint 3	COM of C_α atoms of residues 1160-1174 of three chains A B C
Joint 4	COM of C_α atoms of residues 11141-1146 of three chains A B C
End Effector	COM of C_α atoms of residues 332-442 of three chains A B C

[a] COM Center of mass

Table 2: Simulation data used in this study

| Source	Length	Description	Code name
Mehdipour lab	3×0.5 μs	Full length glycosylated spike	$Mehdipour_{Glyc}$
Mehdipour lab	3×0.5 μs	Full length nonglycosylated spike	$Mehdipour_{Noglyc}$
Hummer lab	2.5 μs	Four copies of Full length glycosylated spike	$Hummer_{Glyc}$
Tajkhorshid lab	5 μs	Full length glycosylated spike	$Tajkhorshid_{Glyc}$
Tajkhorshid lab	5 μs	Full length nonglycosylated spike	$Tajkhorshid_{Noglyc}$
Im lab	16×1.28 μs	Full length glycosylated spike	Im_{Glyc}
Klauda lab	1 μs	Full length glycosylated spike	$Klauda_{glyc}$
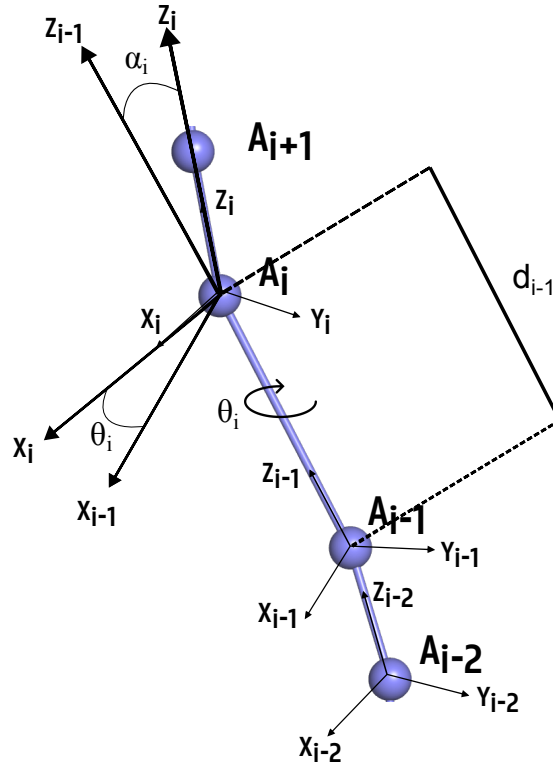
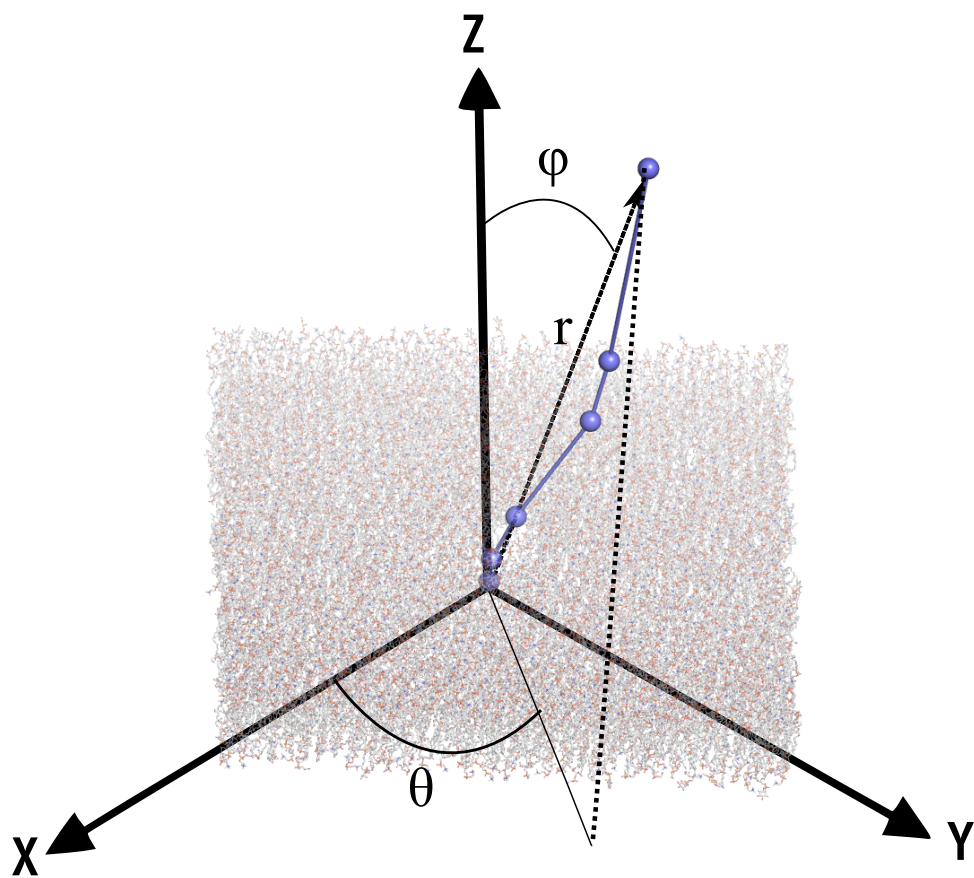Figure S 1: **Denavit-Hartenberg (DH) convention and parameters**.

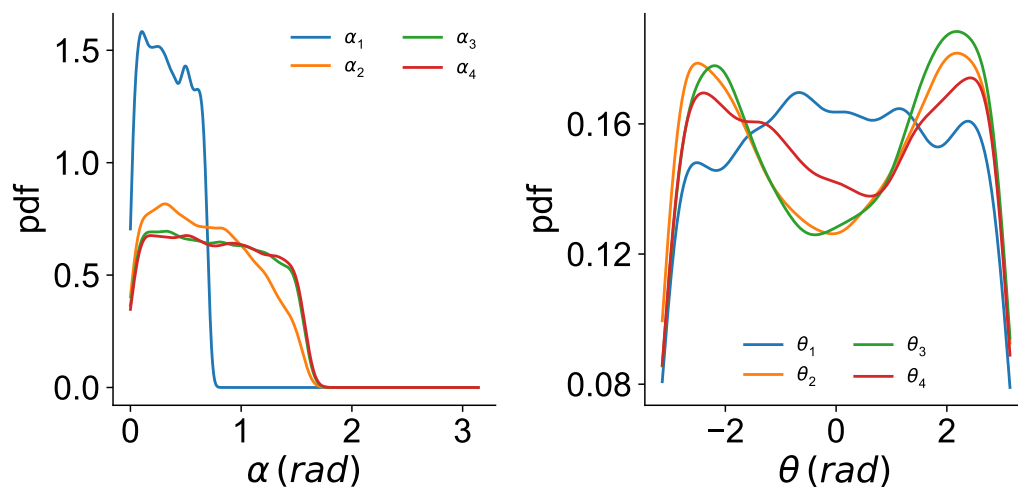Figure S 2: **Spherical coordinates convention and parameters**.

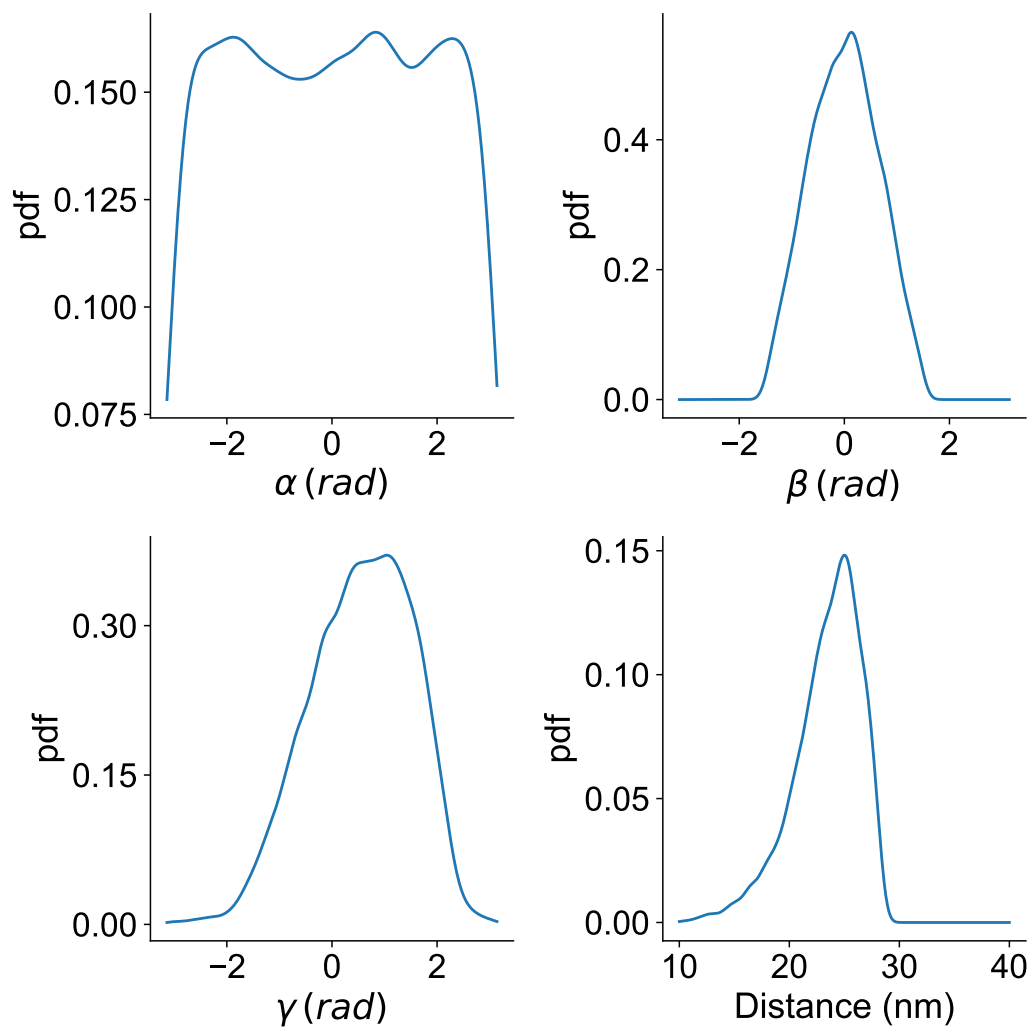Figure S 3: **Distribution of Denavit-Hartenberg (DH) parameters for the generated robotic arm of spike**.

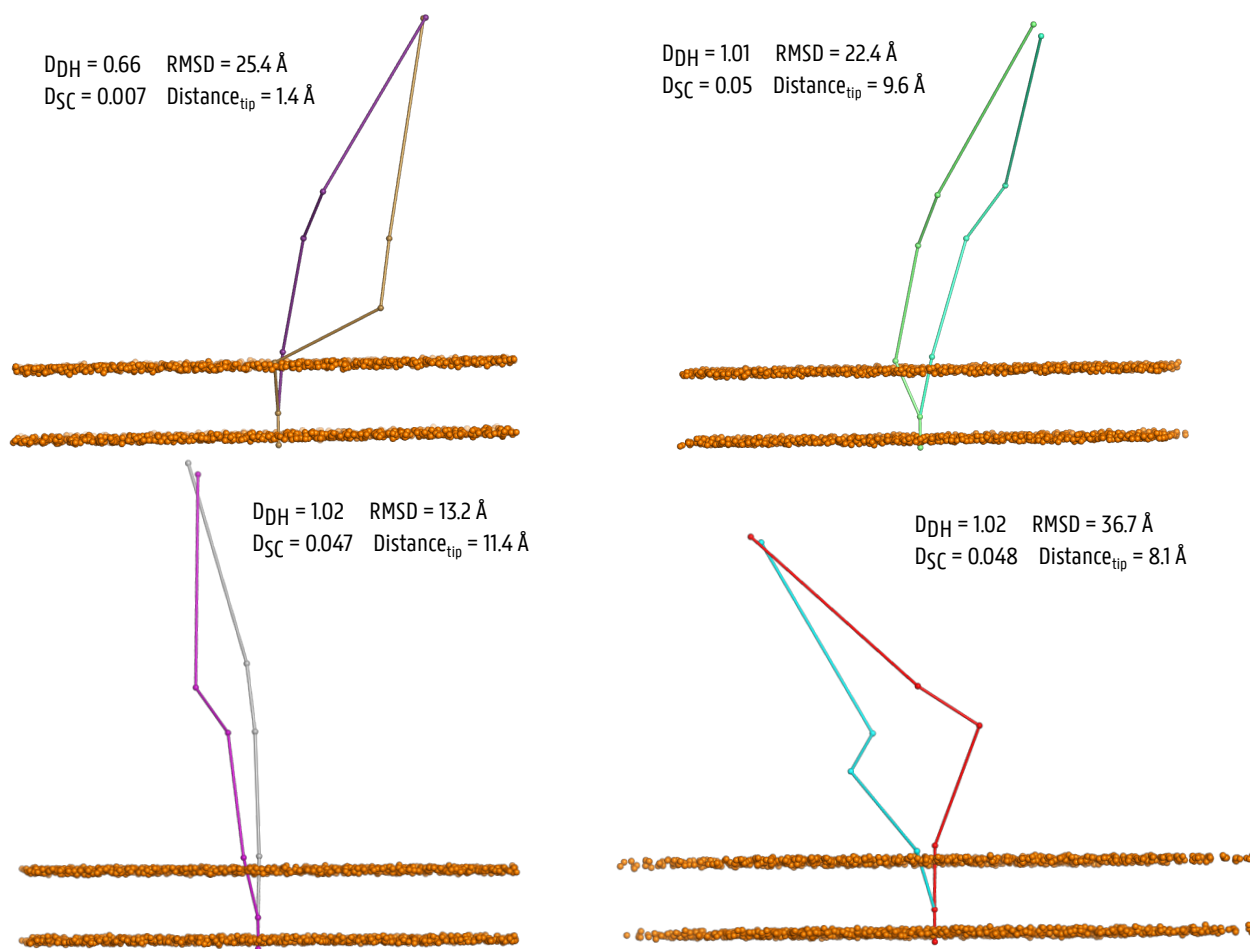Figure S 4: **Spherical coordinate parameters for the generated robotic arm of spike**.

Figure S 5: **Generated robotic arms with similar SC parameters and tip point position.**