Features	Definition	Access
$\varphi_{C-C-C-C}(Biaryl_{GS})$	The dihedral of ground state aldehyde substrate	Based on xTB optimized geometries
$\Delta G^{\ddagger}_{rot}(Biaryl_{GS})$	The rotational free energy of ground state aldehyde substrate	xTB calculation based on xTB optimized geometries
$\theta_{N-Pd-O}(TDG^{b}_{GS})$	The bite angle between palladium and amino acid of ground state palladium complex with base fragment	Based on xTB optimized geometries
$\theta_{N-Pd-O}(TDG_{GS})$	The bite angle between palladium and amino acid of ground state palladium complex without base fragment	Based on xTB optimized geometries
$\%V^{3.5Å}_{Bur}(TDG^{R}_{CH})$	The buried volume of chiral carbon at amino acid of palladium complex derived from (*R*)-C–H bond activation, sphere radius = 3.5Å	Calculation based on xTB optimized geometries
$\%V^{3.5Å}_{Bur}(TDG^{S}_{CH})$	The buried volume of chiral carbon at amino acid of palladium complex derived from (*S*)-C–H bond activation, sphere radius = 3.5Å	Calculation based on xTB optimized geometries
$\%V^{3.5Å}_{Bur}(TDG^{b}_{GS})$	The buried volume of chiral carbon at amino acid of ground state palladium complex with base fragment, sphere radius = 3.5Å	Calculation based on xTB optimized geometries
$\%V^{3.5Å}_{Bur}(TDG^{R}_{AI})$	The buried volume of chiral carbon at amino acid of palladium complex derived from (*R*)-alkene insertion, sphere radius = 3.5Å	Calculation based on xTB optimized geometries
$\%V^{3.5Å}_{Bur}(TDG^{S}_{AI})$	The buried volume of chiral carbon at amino acid of palladium complex derived from (*S*)-alkene insertion, sphere radius = 3.5Å	Calculation based on xTB optimized geometries
$\%V^{3.5Å}_{Bur}(TDG_{GS})$	The buried volume of chiral carbon at amino acid of ground state palladium complex without base fragment, sphere radius = 3.5Å	Calculation based on xTB optimized geometries
$B_1(TDG^{R}_{CH})$	Sterimol parameter B_1 of palladium complex derived from (*R*)-C–H bond activation, dummy index: chiral carbon, attached index: atom in substituent group attach to chiral carbon	Calculation based on xTB optimized geometries
$B_1(TDG^{S}_{CH})$	Sterimol parameter B_1 of palladium complex derived from (*S*)-C–H bond activation, dummy index: chiral carbon, attached index: atom in substituent group attach to chiral carbon	Calculation based on xTB optimized geometries
$B_1(TDG^{b}_{GS})$	Sterimol parameter B_1 of ground state palladium complex with base fragment, dummy index: chiral carbon, attached index: atom in substituent group attach to chiral carbon	Calculation based on xTB optimized geometries
$B_1(TDG^{R}_{AI})$	Sterimol parameter B_1 of palladium complex derived from (*R*)-alkene insertion, dummy index: chiral carbon, attached index: atom in substituent group attach to chiral carbon	Calculation based on xTB optimized geometries
$B_1(TDG^{S}_{AI})$	Sterimol parameter B_1 of palladium complex derived from (*S*)-alkene insertion, dummy index: chiral carbon, attached index: atom in substituent group attach to chiral carbon	Calculation based on xTB optimized geometries
$B_1(TDG_{GS})$	Sterimol parameter B_1 of ground state palladium complex without base fragment, dummy index: chiral carbon, attached	Calculation based on xTB optimized geometries

	index: atom in substituent group attach to chiral carbon	
$B_5(TDG_{CH}^R)$	Sterimol parameter B_5 of palladium complex derived from (R)-C–H bond activation, dummy index: chiral carbon, attached index: atom in substituent group attach to chiral carbon	Calculation based on xTB optimized geometries
$B_5(TDG_{CH}^S)$	Sterimol parameter B_5 of palladium complex derived from (S)-C–H bond activation, dummy index: chiral carbon, attached index: atom in substituent group attach to chiral carbon	Calculation based on xTB optimized geometries
$B_5(TDG_{GS}^b)$	Sterimol parameter B_5 of ground state palladium complex with base fragment, dummy index: chiral carbon, attached index: atom in substituent group attach to chiral carbon	Calculation based on xTB optimized geometries
$B_5(TDG_{AI}^R)$	Sterimol parameter B_5 of palladium complex derived from (R)-alkene insertion, dummy index: chiral carbon, attached index: atom in substituent group attach to chiral carbon	Calculation based on xTB optimized geometries
$B_5(TDG_{AI}^S)$	Sterimol parameter B_5 of palladium complex derived from (S)-alkene insertion, dummy index: chiral carbon, attached index: atom in substituent group attach to chiral carbon	Calculation based on xTB optimized geometries
$B_5(TDG_{GS})$	Sterimol parameter B_5 of ground state palladium complex without base fragment, dummy index: chiral carbon, attached index: atom in substituent group attach to chiral carbon	Calculation based on xTB optimized geometries
$L(TDG_{CH}^R)$	Sterimol parameter L of palladium complex derived from (R)-C–H bond activation, dummy index: chiral carbon, attached index: atom in substituent group attach to chiral carbon	Calculation based on xTB optimized geometries
$L(TDG_{CH}^S)$	Sterimol parameter L of palladium complex derived from (S)-C–H bond activation, dummy index: chiral carbon, attached index: atom in substituent group attach to chiral carbon	Calculation based on xTB optimized geometries
$L(TDG_{GS}^b)$	Sterimol parameter L of ground state palladium complex with base fragment dummy index: chiral carbon, attached index: atom in substituent group attach to chiral carbon	Calculation based on xTB optimized geometries
$L(TDG_{AI}^R)$	Sterimol parameter L of palladium complex derived from (R)-alkene insertion, dummy index: chiral carbon, attached index: atom in substituent group attach to chiral carbon	Calculation based on xTB optimized geometries
$L(TDG_{AI}^S)$	Sterimol parameter L of palladium complex derived from (S)-alkene insertion, dummy index: chiral carbon, attached index: atom in substituent group attach to chiral carbon	Calculation based on xTB optimized geometries
$L(TDG_{GS})$	Sterimol parameter L of ground state palladium complex without base fragment dummy index: chiral carbon, attached index: atom in substituent group attach to chiral carbon	Calculation based on xTB optimized geometries