Table S6D. Intramolecular Heck reaction dataset divided into test dataset in our research for transformer-baseline and transformer-transfer learning models (Dataset for testing in experiment 1)

Reaction ID	Reaction SMILES
1	C=CC(C)(C)Nc1nc(Cl)ncc1Br>>C=C1c2cnc(Cl)nc2NC1(C)C
2	C=CCC(CCBr)c1ccc(OC)cc1>>C=C1CCC(c2ccc(OC)cc2)C1
3	C=CCn1c(N(c2ccc(F)cc2I)S(=O)(=O)c2cccs2)cc2cc(C)ccc21>>Cc1ccc2c(c1)cc1n2C/C=C\c2cc(F)ccc2N1S(=O)(=O)c1cccs1
4	C=CCC(O)c1cc2cc(C)ccc2nc1Cl>>C=C1CC(O)c2cc3cc(C)ccc3nc21
5	C=CCc1c(OCc2ccccc2Br)c(=O)n(C)c2ccccc12>>C=C1Cc2c(c(=O)n(C)c3ccccc23)OCc2ccccc21
6	C=CCN(CC1=C(Br)CCc2ccccc21)c1ccc(Cl)cc1>>C=C1CN(c2ccc(Cl)cc2)CC2=C1CCc1ccccc12
7	COC(=O)/C=C/Oc1ccccc1-c1cc(C)c(C)cc1Br>>COC(=O)/C=C1/Oc2ccccc2-c2cc(C)c(C)cc21
8	C=CCC(O)c1cc2cccc(C)c2nc1Cl>>C=C1CC(O)c2cc3cccc(C)c3nc21
9	C=CC(=O)OCCCCC(=O)CCCC(CCc1cccnc1)OC(=O)[C@@H]1CCCCN1C(=O)C(=O)c1cccc(I)c1>>O=C1CCCCOC(=O)/C=C/c2cccc(c2)C(=O)C(=O)N2CCCC[C@H]2C(=O)OC(CCc2cccnc2)CCC1
10	Cc1ccc(/C=C/C(=O)O/C(=C\I)C2CC2)cc1>>Cc1ccc(/C=C2\C=C(C3CC3)OC2=O)cc1
11	C=CCN(Cc1ccc(OC)cc1)Cc1cc2ccccc2nc1Cl>>C=C1CN(Cc2ccc(OC)cc2)Cc2cc3ccccc3nc21
12	C=CCN(Cc1cc2ccc(C)cc2nc1Cl)c1ccc(OC)cc1>>C=C1CN(c2ccc(OC)cc2)Cc2cc3ccc(C)cc3nc21
13	C=CCC(CCBr)c1ccc(C(F)(F)F)cc1>>C=C1CCC(c2ccc(C(F)(F)F)cc2)C1
14	C=Cc1cccc(C(=O)O[C@H]2[C@H]3[C@](C)(C(=O)[C@H](OC(C)=O)C4=C(C)[C@@H](OC(=O)[C@H](O[Si](CC)(CC)CC)[C@@H](NC(=O)c5cccc(I)c5)c5ccccc5)C[C@]2(O)C4(C)C)[C@@H](O[Si](CC)(CC)CC)C[C@H]2OC[C@]23OC(C)=O)c1>>C=C1c2cccc(c2)C(=O)N[C@@H](c2ccccc2)[C@@H](O[Si](CC)(CC)CC)C(=O)O[C@H]2C[C@@]3(O)[C@@H](OC(=O)c4cccc1c4)[C@H]1[C@](C)(C(=O)[C@H](OC(C)=O)C(=C2C)C3(C)C)[C@@H](O[Si](CC)(CC)CC)C[C@H]2OC[C@]21OC(C)
15	C=Cc1cc(C(C)=O)ccc1N(C)C(=O)c1ccccc1I>>C=C1c2ccccc2C(=O)N(C)c2ccc(C(C)=O)cc21
16	C=CC(=O)N(C)[C@@H](CO)Cc1ccc(OC)cc1Br>>C=C1C(=O)N(C)[C@@H](CO)Cc2ccc(OC)cc21
17	C=C(C(=O)OC)N(CCCCCc1ccccc1I)C(=O)OC(C)(C)C>>COC(=O)/C1=C/c2ccccc2CCCCCN1C(=O)OC(C)(C)C
18	C=CCCCC(=O)N(Cc1ccccc1)c1ccccc1I>>C=C1CCCC(=O)N(Cc2ccccc2)c2ccccc21
19	C=CCN(CCc1ccc(C(F)(F)F)cc1I)C(=O)C(F)(F)F>>C=C1CN(C(=O)C(F)(F)F)CCc2ccc(C(F)(F)F)cc21
20	C=C[C@@H](O[Si](C)(C)C(C)(C)C)[C@@H](CCCC)[C@@H](C/C(I)=C/CO)O[Si](C)(C)C(C)(C)C>>C=C1/C(=C\CO)C[C@@H](O[Si](C)(C)C(C)(C)C)[C@H](CCCC)[C@@H]1O[Si](C)(C)C(C)(C)C
21	C=CCn1c(N(c2ccc(C)cc2I)S(=O)(=O)c2cccs2)cc2ccccc21>>Cc1ccc2c(c1)/C=C\Cn1c(cc3ccccc31)N2S(=O)(=O)c1cccs1
22	C=CC(=O)NC(CC(=O)N[C@@H](Cc1ccccc1)C(=O)N[C@@H](CC(C)C)C(=O)NCc1cccc(Br)c1)c1ccccc1>>CC(C)C[C@@H]1NC(=O)[C@H](Cc2ccccc2)NC(=O)CC(c2ccccc2)NC(=O)/C=C/c2cccc(c2)
23	C=CCC(O)c1ccncc1Br>>C=C1CC(O)c2ccncc21
24	C=CCCCNc1ccccc1Br>>C=C1CCCNc2ccccc21
25	C=C[Si](C)(C)c1cc(OC)c(OC)cc1-c1cc(OC)c(OC)cc1Br>>C=C1c2cc(OC)c(OC)cc2-c2cc(OC)c(OC)cc2[Si]1(C)C
26	C=C[C@@H](O[Si](C)(C)C(C)(C)C)[C@H](OCCCO[Si](c1ccccc1)(c1ccccc1)C(C)(C)C)[C@@H](C/C(I)=C/CO)O[Si](C)(C)C(C)(C)C>>C=C1/C(=C\CO)C[C@@H](O[Si](C)(C)C(C)(C)C)[C@@H](OCCCO[Si](c2ccccc2)(c2ccccc2)C(C)(C)C)[C@@H]1O[Si](C)(C)C(C)(C)C
27	C=CC(C)c1ccc2ccccc2c1OS(=O)(=O)c1ccccc1Br>>C=C1c2ccccc2S(=O)(=O)Oc2c(ccc3ccccc23)C1C
28	C=C[C@@H](O[Si](C)(C)C(C)(C)C)[C@@H](Cc1ccccc1)[C@@H](CC(I)=CCO)O[Si](C)(C)C(C)(C)C>>C=C1C(=CCO)C[C@@H](O[Si](C)(C)C(C)(C)C)[C@H](Cc2ccccc2)[C@@H]1O[Si](C)(C)C(C)
29	C=CCCN(c1ccccc1[N+](=O)[O-])S(=O)(=O)c1ccccc1Br>>C=C1CCN(c2ccccc2[N+](=O)[O-])S(=O)(=O)c2ccccc21
30	C=CCc1c(OCc2ccccc2Br)c(=O)n(C)c(=O)n1C>>Cn1c2c(c(=O)n(C)c1=O)OCc1ccccc1/C=C\C2
31	C=CC[C@@H](N[S@@](=O)C(C)(C)C)c1c(F)cccc1Br>>C=C1C[C@@H](N[S@@](=O)C(C)(C)C)c2c(F)cccc21
32	C=CCC(OC)c1cc2ccccc2nc1Cl>>C=C1CC(OC)c2cc3ccccc3nc21
33	C=C[C@H](O[Si](C)(C)C(C)(C)C)[C@H](OCCCO[Si](c1ccccc1)(c1ccccc1)C(C)(C)C)[C@@H](C/C(I)=C/CO)O[Si](C)(C)C(C)(C)C>>C=C1/C(=C\CO)C[C@@H](O[Si](C)(C)C(C)(C)C)[C@@H](OCCCO[Si](c2ccccc2)(c2ccccc2)C(C)(C)C)[C@H]1O[Si](C)(C)C(C)(C)C
34	C=CC(=O)NC[C@@H](OC)[C@H](OC)c1ccccc1NC(=O)[C@H](CC(C)C)NC(=O)c1cccc(Br)c1>>CO[C@@H]1CNC(=O)/C=C/c2cccc(c2)C(=O)N[C@@H](CC(C)C)C(=O)Nc2ccccc2[C@H]1OC

35 C=C[C@H]1[C@@H]2[C@H](CN1c1cc(C(=O)OC)cc(OCc3ccccc3)c1I)N2C(=O)OC(C)(C)C>>C=C1c2c(OCc3ccccc3)cc(C(=O)OC)cc2N2C[C@H]3[C@@H]([C@H]12)N3C(=O)OC(C)(C)C
36 C=CCCOCC1=C(Br)CCc2ccccc21>>C=C1CCOCC2=C1CCc1ccccc12
37 C=CCCOCC1=C(Br)c2ccccc2C(C)C1>>C=C1CCOCC2=C1c1ccccc1C(C)C2
38 C=Cc1ccc(OC)c(Nc2nc(Nc3ccc(N4CCOCC4)c(Br)c3)ncc2Cl)c1>>COc1ccc2cc1Nc1nc(ncc1Cl)Nc1ccc(N3CCOCC3)c(c1)/C=C\2
39 C=CC(F)(F)Oc1ccc(OC)cc1Br>>C=C1c2cc(OC)ccc2OC1(F)F
40 C=CCC1c2[nH]c3ccccc3c2CCN1CC(=C)I>>C=C1CC2c3[nH]c4ccccc4c3CCN2CC1=C
41 C=CS(=O)(=O)N(CC(=C)Br)Cc1ccccc1>>C=C1C=CS(=O)(=O)N(Cc2ccccc2)C1
42 C=CCn1c(N(c2ccc(F)cc2I)S(=O)(=O)c2cccs2)cc2ccccc21>>O=S(=O)(c1cccs1)N1c2ccc(F)cc2/C=C\Cn2c1cc1ccccc12
43 C=CCN(CC1=C(Br)c2ccccc2CC1)c1ccc(C)cc1>>C=C1CN(c2ccc(C)cc2)CC2=C1c1ccccc1CC2
44 C=CCOCc1ccc2ccccc2c1Br>>C=C1COCc2ccc3ccccc3c21
45 C=C(C(=O)OCC)c1ccccc1CN(C(=O)C(F)(F)F)c1ccccc1Br>>CCOC(=O)/C1=C/c2ccccc2N(C(=O)C(F)(F)F)Cc2ccccc21
46 C=CC(OCC(=C)Br)c1cccc(Cl)c1>>C=C1COC(c2cccc(Cl)c2)C1=C
47 C=C[C@@H](O[Si](C)(C)C(C)(C)C)[C@@H](C)[C@@H](C/C(I)=C/CO)O[Si](C)(C)C(C)(C)C>>C=C1/C(=C\CO)C[C@@H](O[Si](C)(C)C(C)(C)C)[C@H](C)[C@@H]1O[Si](C)(C)C(C)(C)C
48 C=CC(CC)(CC)C(=O)Nc1ccc(C(F)(F)F)cc1Br>>C=C1c2cc(C(F)(F)F)ccc2NC(=O)C1(CC)CC
49 C=Cc1ccccc1N(C)C(=O)c1ccccc1I>>C=C1c2ccccc2C(=O)N(C)c2ccccc21
50 C=Cc1cc(Nc2ncc(Cl)c(Nc3cc(Br)ccc3C(=O)OC)n2)ccc1N1CCN(C)CC1>>COC(=O)c1ccc2cc1Nc1nc(ncc1Cl)Nc1ccc(N3CCN(C)CC3)c(c1)/C=C\2
51 C=CC(Cn1c(Br)c(-c2ccc(Oc3ccccc3)cc2)c2c(N)ncnc21)NC(=O)OC(C)(C)C>>C=C1c2c(-c3ccc(Oc4ccccc4)cc3)c3c(N)ncnc3n2CC1NC(=O)OC(C)(C)C
52 C=Cc1ccccc1CO[Si](Cl)(C(C)C)C(C)C>>CC(C)[Si]1(C(C)C)C/C=C\c2ccccc2CO1
53 C=Cc1cc(CCCCCC)ccc1N(C)C(=O)c1ccccc1I>>C=C1c2ccccc2C(=O)N(C)c2ccc(CCCCCC)cc21
54 C=CCC[C@@H](C=C)COc1ccccc1Br>>C=CCC[C@@H]1COc2ccccc2C1=C
55 C=Cc1cccc(Nc2nc(Nc3ccc(N4CCN(C)CC4)c(Br)c3)ncc2Cl)c1>>CN1CCN(c2ccc3cc2/C=C\c2cccc(c2)Nc2nc(ncc2Cl)N3)CC1