Table S6C. Intramolecular Heck reaction dataset divided into validation dataset in our research for transformer-baseline and transformer-transfer learning models (Dataset for validation in experiment 1)

Reaction ID	Reaction SMILES
1	C=CCN(C)C(=O)C1(CC(=C)Br)CC/C(=C\c2ccccc2)C1=O>>C=C1CN(C)C(=O)C2(CC/C(=C\c3ccccc3)C2=O)CC1=C
2	C=CCc1c(N(C)C(=O)Cc2ccccc2I)ccc2c1ccc(=O)n2C>>C=C1Cc2c(ccc3c2ccc(=O)n3C)N(C)C(=O)Cc2ccccc21
3	C=CCc1cccc(F)c1N(Cc1cc(OC)ccc1Br)S(=O)(=O)c1ccc(C)cc1>>C=C1Cc2cccc(F)c2N(S(=O)(=O)c2ccc(C)cc2)Cc2cc(OC)ccc21
4	C=CCOCc1nnn(Cc2ccc(C)cc2)c1I>>C=C1COCc2nnn(Cc3ccc(C)cc3)c21
5	C=CCN(CC1=C(Br)CCCCC1)c1ccc(Cl)cc1>>C=C1CN(c2ccc(Cl)cc2)CC2=C1CCCCC2
6	C=CCCCOc1cccnc1Br>>C=C1CCCOc2cccnc21
7	C=CCCOCC1=C(Br)c2cc(OC)ccc2CC1>>C=C1CCOCC2=C1c1cc(OC)ccc1CC2
8	C=C[C@@H](O[Si](C)(C)C(C)(C)C)[C@@H](c1ccccc1)[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](c2ccccc2)[C@@H]1O[Si](C)(C)C(C)(
9	C=CC(F)(F)Oc1ccccc1Br>>C=C1c2ccccc2OC1(F)F
10	C=CC1CCCN1Cc1ccccc1I>>C=C1c2ccccc2CN2CCCC12
11	C=CC(=O)OCCCCC(CCc1cccnc1)OC(=O)[C@@H]1CCCCN1C(=O)C(=O)c1cccc(I)c1>>O=C1/C=C/c2cccc(c2)C(=O)C(=O)N2CCCC[C@H]2C(=O)OC(CCc2cccnc2)CCCCO1
12	C=CCCC(=O)N(Cc1ccccc1)c1ccccc1I>>C=C1CCC(=O)N(Cc2ccccc2)c2ccccc21
13	C=CC[C@H](N[S@](=O)C(C)(C)C)c1ccccc1Br>>C=C1C[C@H](N[S@](=O)C(C)(C)C)c2ccccc21
14	C=CCN(C(=O)c1ccc2ccccc2c1Br)C(C(=O)NC(C)(C)C)c1ccc(C)cc1>>C=C1CN(C(C(=O)NC(C)(C)C)c2ccc(C)cc2)C(=O)c2ccc3ccccc3c21
15	C=CCCCC(O)C=C(Br)c1ccc(C)cc1>>C=C1CCCC(O)C=C1c1ccc(C)cc1
16	C=CCn1c(-c2ccc3cc(OC)ccc3c2Br)nc2ccccc21>>C=C1Cn2c(nc3ccccc32)-c2ccc3cc(OC)ccc3c21
17	C=CCOCc1c(Br)c(OC)c2ccccc2c1OC>>C=C1COCc2c1c(OC)c1ccccc1c2OC
18	C=C[C@@H](O[Si](C)(C)C(C)(C)C)[C@@H](CCCO[Si](C)(C)C(C)(C)C)[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](CCCO[Si](C)(C)C(C)(C)C)[C@@H]1O[Si](C)(C)C(C)(C)C
19	C=COC(=O)c1ccccc1Br>>C=C1OC(=O)c2ccccc21
20	C=CCc1cc(C)ccc1N(C(=O)c1ccccc1I)S(=O)(=O)c1ccc(C)cc1>>C=C1Cc2cc(C)ccc2N(S(=O)(=O)c2ccc(C)cc2)C(=O)c2ccccc21
21	C=CCn1c(N(c2ccc(F)cc2I)S(=O)(=O)c2ccc(C)cc2)cc2cc(OC)ccc21>>COc1ccc2c(c1)cc1n2C/C=C\c2cc(F)ccc2N1S(=O)(=O)c1ccc(C)cc1
22	C=CCCc1c(Br)cncc1C1=N[C@H](c2ccccc2)CO1>>C=C1CCc2c1cncc2C1=N[C@H](c2ccccc2)CO1
23	C=CCO[C@H](CSc1ccccc1Br)[C@H]1O[C@@H]2OC(C)(C)O[C@@H]2[C@H]1OCc1ccccc1>>C=C1CO[C@@H]([C@H]2O[C@@H]3OC(C)(C)O[C@@H]3[C@H]2OCc2ccccc2)CSc2ccccc21
24	C=CCN(Cc1ccccc1I)S(=O)(=O)c1ccc(C)cc1>>C=C1CN(S(=O)(=O)c2ccc(C)cc2)Cc2ccccc21
25	C=CCN(CC1=C(Br)CCCC1)c1ccc(C)cc1>>C=C1CN(c2ccc(C)cc2)CC2=C1CCCC2
26	C=CCCCC(O)C1=C(Br)CCCCC1>>C=C1CCCC(O)C2=C1CCCCC2
27	C=CCC(c1ccccc1)N(C)c1ccccc1I>>C=C1CC(c2ccccc2)N(C)c2ccccc21
28	C=C[C@H]1O[C@@H]2OC(C)(C)O[C@@H]2[C@@H]1N(Cc1ccccc1Br)S(=O)(=O)c1ccc(C)cc1>>C=C1c2ccccc2CN(S(=O)(=O)c2ccc(C)cc2)[C@@H]2[C@@H]1O[C@@H]1OC(C)(C)O[C@@H]12
29	C=CCC(NCc1ccc(C)cc1Br)(C(=O)OC)C(C)C>>C=C1CC(C(=O)OC)(C(C)C)NCc2ccc(C)cc21
30	C=CCOc1ccc(C(NC(=O)c2ccccc2)C(=O)OC)cc1I>>C=C1COc2ccc(C(NC(=O)c3ccccc3)C(=O)OC)cc
31	C=CCc1cc2c(C)cc(=O)oc2c(C)c1OCc1ccccc1I>>C=C1Cc2cc3c(C)cc(=O)oc3c(C)c2OCc2ccccc21
32	C=CC(COc1ccccc1I)NC(=O)OCc1ccccc1>>C=C1c2ccccc2OCC1NC(=O)OCc1ccccc1
33	C=Cc1cc(OC)ccc1OS(=O)(=O)c1ccccc1Br>>COc1ccc2c(c1)/C=C\c1ccccc1S(=O)(=O)O2
34	C=CCc1cccc(C)c1N(C(=O)c1ccccc1I)S(=O)(=O)c1ccc(C)cc1>>C=C1Cc2cccc(C)c2N(S(=O)(=O)c2ccc(C)cc2)C(=O)c2ccccc21
35	C=CCc1c(OCc2cc(OC)ccc2Br)cc(C)n(C)c1=O>>C=C1Cc2c(cc(C)n(C)c2=O)OCc2cc(OC)ccc21
36	C=CCC(O)c1cc2ccc(OC)cc2nc1Cl>>C=C1CC(O)c2cc3ccc(OC)cc3nc21
37	C=CCCN([C@@H](CC(C)C)C(=O)OC)S(=O)(=O)c1ccccc1Br>>C=C1CCN([C@@H](CC(C)C)C(=O)OC)S(=O)(=O)c2ccccc21
38	C=CCO[C@H]1[C@H](Sc2ccccc2Br)O[C@H](COCc2ccccc2)[C@@H](OCc2ccccc2)[C@@H]1OCc1ccccc1>>C=C1CO[C@H]2[C@@H](O[C@H](COCc3ccccc3)[C@@H](OCc3ccccc3)[C@@H]2OCc2ccccc2)Sc2ccccc21

39 C=CCc1ccccc1N(Cc1cc(OC)ccc1Br)S(=O)(=O)c1ccc(C)cc1>>C=C1Cc2ccccc2N(S(=O)(=O)c2ccc(C)cc2)Cc2cc(OC)ccc21

40 C=CCN1c2c(Br)cc([N+](=O)[O-])cc2C(=O)N2C1C(C)(C)SC2(C)C>>C=C1CN2c3c1cc([N+](=O)[O-])cc3C(=O)N1C2C(C)(C)SC1(C)C

41 C=CCc1ccccc1N(C(=O)c1ccccc1I)S(=O)(=O)c1ccc(C)cc1>>C=C1Cc2ccccc2N(S(=O)(=O)c2ccc(C)cc2)C(=O)c2ccccc21

42 C=CC(OCC(=C)Br)c1cccc(OC)c1>>C=C1COC(c2cccc(OC)c2)C1=C

43 C=CC(F)(F)Oc1ccc(C#N)cc1Br>>C=C1c2cc(C#N)ccc2OC1(F)F

44 C=CC[C@@H](N[S@@](=O)C(C)(C)C)c1cc(F)ccc1Br>>C=C1C[C@@H](N[S@@](=O)C(C)(C)C)c2cc(F)ccc21

45 C=CCC(CCBr)c1ccccc1>>C=C1CCC(c2ccccc2)C1

46 C=C[C@@H](Cn1c(Br)c(-c2ccc(C(=O)NCc3ccccc3)cc2)c2c(N)ncnc21)NC(=O)OC(C)(C)C>>C=C1c2c(-

47 C=CCC(CCCl)CCCCCCCCC>>C=C1CCC(CCCCCCCC)C1

48 C=CCc1c(N(C)C(=O)c2ccccc2I)ccc2c1ccc(=O)n2C>>C=C1Cc2c(ccc3c2ccc(=O)n3C)N(C)C(=O)c2ccccc21

49 C=CCc1c(N(CC)C(=O)c2ccccc2I)ccc2oc(=O)ccc12>>C=C1Cc2c(ccc3oc(=O)ccc23)N(CC)C(=O)c2ccccc21

50 C=CCC(OCC(=C)Br)c1ccccc1>>C=C1COC(c2ccccc2)CC1=C

51 C=Cc1cc(C(C)(C)C)ccc1N(C)C(=O)c1ccccc1I>>C=C1c2ccccc2C(=O)N(C)c2ccc(C(C)(C)C)cc21

52 C=C(C(=O)OCC)c1ccccc1CN(C(=O)C(F)(F)F)c1ccccc1I>>CCOC(=O)/C1=C/c2ccccc2N(C(=O)C(F)(F)F)Cc2ccccc21

53 C=CCN(CCI)S(=O)(=O)c1ccccc1Br>>C=C1CCN(S(=O)(=O)c2ccccc2Br)C1

54 C=Cc1cc(O)ccc1N(C)C(=O)c1ccccc1I>>C=C1c2ccccc2C(=O)N(C)c2ccc(O)cc21

55 C=Cc1ccccc1OCc1ccccc1Br>>C1=C\c2ccccc2OCc2ccccc2/1