Table S8D.Heck reaction database of trisubstituted alkene alkene as reactant

Reaction ID	Reaction SMILES
1	Brc1ccc(I)cc1.CCOC(=O)/C(F)=C\CCc1ccccc1>>CCOC(=O)/C(F)=C(\CCc1ccccc1)c1ccc(Br)cc1
2	CC(=O)c1ccc(I)cc1.CCOC(=O)/C(F)=C\CCc1ccccc1>>CCOC(=O)/C(F)=C(\CCc1ccccc1)c1ccc(C(C)=O)cc1
3	CCOC(=O)/C(F)=C\CCc1ccccc1.COC(=O)c1ccccc1I>>CCOC(=O)/C(F)=C(\CCc1ccccc1)c1ccccc1C(=O)OC
4	COc1ccc(I)cc1.Cc1ccc(S(=O)(=O)/C=C2/C(F)(F)C2(C)C(C)(C)C)cc1>>COc1ccc(/C(=C2\C(F)(F)C2(C)C(C)(C)C)S(=O)(=O)c2ccc(C)cc2)cc1
5	Cc1ccc(I)cc1.Cc1ccc(S(=O)(=O)/C=C2\C(C)(C)C2(F)F)cc1>>Cc1ccc(/C(=C2/C(C)(C)C2(F)F)S(=O)(=O)c2ccc(C)cc2)cc1
6	CCC1(C)/C(=C\S(=O)(=O)c2ccc(C)cc2)C1(F)F.COc1ccc(I)cc1>>CCC1(C)/C(=C(/c2ccc(OC)cc2)S(=O)(=O)c2ccc(C)cc2)C1(F)F
7	Cc1ccc(S(=O)(=O)/C=C2\C(C)(C)C2(F)F)cc1.Ic1ccccc1>>Cc1ccc(S(=O)(=O)/C(=C2\C(C)(C)C2(F)F)c2ccccc2)cc1
8	Cc1ccc(S(=O)(=O)/C=C2\C(C)(C)C2(F)F)cc1.Clc1ccc(I)cc1>>Cc1ccc(S(=O)(=O)/C(=C2\C(C)(C)C2(F)F)c2ccc(Cl)cc2)cc1
9	Brc1ccc(OCCCCc2ccccc2)cc1.C/C=C(\CCO)C(=O)OCC>>CCOC(=O)/C(CCO)=C(\C)c1ccc(OCCCCc2ccccc2)cc1
10	CC/C(=C\c1ccccc1)c1ccccc1.CN(C)CCOc1ccc(Br)cc1>>CC/C(=C(\c1ccccc1)c1ccc(OCCN(C)C)cc1)c1ccccc1
11	COc1ccc(I)cc1.Cc1ccc(S(=O)(=O)/C=C2\C(C)(C)C2(F)F)cc1>>COc1ccc(/C(=C2/C(C)(C)C2(F)F)S(=O)(=O)c2ccc(C)cc2)cc1
12	CCOC(=O)/C(F)=C\CCc1ccccc1.Ic1ccccc1>>CCOC(=O)/C(F)=C(\CCc1ccccc1)c1ccccc1
13	COc1ccc(I)cc1.Cc1ccc(S(=O)(=O)/C=C2/C(F)(F)C23CCCCC3)cc1>>COc1ccc(/C(=C2\C(F)(F)C23CCCCC3)S(=O)(=O)c2ccc(C)cc2)cc1
14	CCOC(=O)/C(F)=C\CCc1ccccc1.COc1ccc(I)cc1>>CCOC(=O)/C(F)=C(\CCc1ccccc1)c1ccc(OC)cc1
15	C/C=C(/NC(=O)OC(C)(C)C)C(=O)OC.CN(C)c1ccc(I)cc1>>COC(=O)/C(NC(=O)OC(C)(C)C)=C(\C)c1ccc(N(C)C)cc1
16	CC=C(c1ccccc1)c1c(OCc2cc(OC)ccc2Br)c(=O)n(C)c(=O)n1C>>COc1ccc2c(c1)COc1c(n(C)c(=O)n(C)c1=O)/C(c1ccccc1)=C\2C
17	C[C@@H](OC(=O)[C@@H](C/C=C1\CCN(c2ccccc2)C1=O)Nc1cc(Cl)ccc1I)C(=O)OC(C)(C)C>>C[C@@H](OC(=O)[C@H]1C/C(=C2/CCN(c3ccccc3)C2=O)c2ccc(Cl)cc2N1)C(=O)OC(C)(C)C
18	CC(C)COC(=O)[C@@H](C)OC(=O)[C@@H](C/C=C1\CCN([13c]2[13cH][13cH][13cH][13cH][13cH][13cH]2)C1=O)Nc1cc(Cl)ccc1I>>CC(C)COC(=O)[C@@H](C)OC(=O)[C@H]1C/C(=C2/CCN([13c]3[13cH][13cH][13cH][13cH][13cH]3)C2=O)c2ccc(Cl)cc2N1
19	COC(=O)/C(=C\CCN(C(=O)OC(C)(C)C)C(=O)c1c(I)c2ccccc2n1C(=O)OC(C)(C)C)OCc1ccccc1>>COC(=O)/C(OCc1ccccc1)=C1/CCN(C(=O)OC(C)(C)C)C(=O)c2c1c1ccccc1n2C(=O)OC(C)(C)C
20	CCOC(=O)[C@@H](C/C=C1\CCN(c2ccccc2)C1=O)Nc1cc(Cl)ccc1I>>CCOC(=O)[C@H]1C/C(=C2/CCN(c3ccccc3)C2=O)c2ccc(Cl)cc2N1
21	CC(C)COC(=O)[C@@H](C)OC(=O)[C@@H](C/C=C1\CCN([14c]2[14cH][14cH][14cH][14cH][14cH][14cH]2)C1=O)Nc1cc(Cl)ccc1I>>CC(C)COC(=O)[C@@H](C)OC(=O)[C@H]1C/C(=C2/CCN([14c]3[14cH][14cH][14cH][14cH][14cH]3)C2=O)c2ccc(Cl)cc2N1
22	CC=C(c1ccccc1)c1c(OCc2ccccc2Br)c(=O)n(C)c(=O)n1C>>C/C1=C(\c2ccccc2)c2c(c(=O)n(C)c(=O)n2C)OCc2ccccc21