

Path #1

Score: 3.00 Estimated cost (\$/g): 729.89

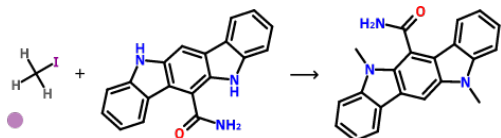
Reaction name: N-heterocycle alkylation

Reaction conditions: K₂CO₃

Solvent: DMF

Alternative Solvent: DMSO

Literature reference: 10.1039/C2OB26456K and 10.1016/j.bmc.2013.12.031

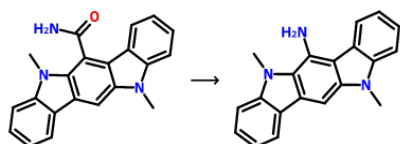


Reaction name: Hofmann rearrangement

Reaction conditions: KOH, Br₂, H₂O, 0 deg C or NaOCl, NaOH, H₂O, from 0 deg C to 75 deg C

Solvent: H₂O

Literature reference: 10.1016/S0022-1139(97)00097-3 and 10.1021/jm000950v and 10.1016/j.bmcl.2012.01.047 (Supporting Information S12) and 10.1002/chem.200390079 and 10.1021/cr040679f (large-scale application)

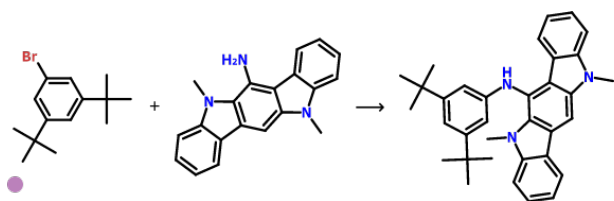


Reaction name: Buchwald-Hartwig Amination with Aromatic Amines

Reaction conditions: [Pd]-catalyst, ligand, Cs₂CO₃, dioxane or [Pd]-catalyst, ligand, KOtBU, dioxane

Solvent: dioxane or toluene

Literature reference: DOI: 10.1021/jo991699y and 10.1002/anie.200601612 and 10.1038/s41586-018-0056-8 and 10.1021/acs.chemrev.6b00512 and 10.1021/op8000146



Path #2

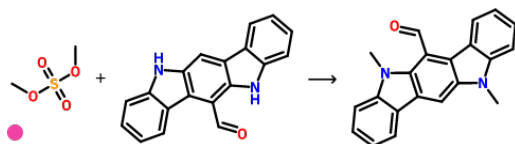
Score: 5.00 Estimated cost (\$/g): 36.22

Reaction name: N-heterocycle alkylation

Reaction conditions: KOH

Solvent: acetone

Literature reference: 10.1016/S0040-4020(98)00865-5

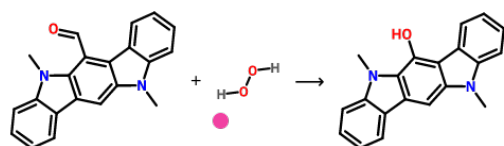


Reaction name: Dakin oxidation

Reaction conditions: UHP, NaOH, MeOH, 0 deg C

Solvent: MeOH

Literature reference: 10.1002/9780470638859.conrr175 ; 10.1021/op400101p

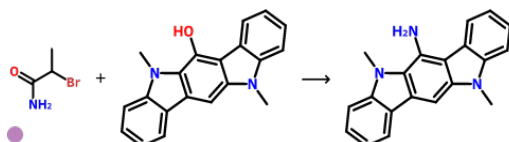


Reaction name: Smiles rearrangement

Reaction conditions: DMSO, KOH then KOH, heating

Solvent: DMSO

Literature reference: 10.1055/s-0033-1338703

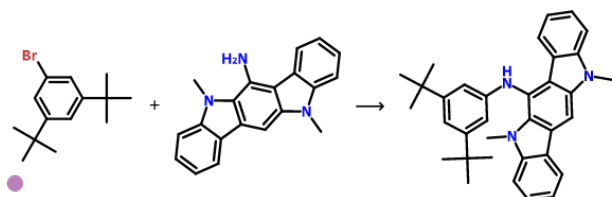


Reaction name: Buchwald-Hartwig Amination with Aromatic Amines

Reaction conditions: [Pd]-catalyst, ligand, Cs2CO3, dioxane or [Pd]-catalyst, ligand, KOtBU, dioxane

Solvent: dioxane or toluene

Literature reference: DOI: 10.1021/jo991699y and 10.1002/anie.200601612 and 10.1038/s41586-018-0056-8 and 10.1021/acs.chemrev.6b00512 and 10.1021/op8000146



Path #3

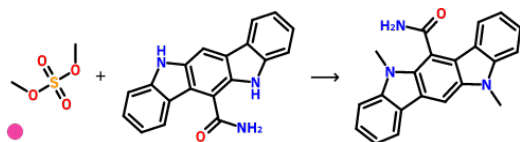
Score: 5.50 Estimated cost (\$/g): 729.75

Reaction name: N-heterocycle alkylation

Reaction conditions: KOH

Solvent: acetone

Literature reference: 10.1016/S0040-4020(98)00865-5

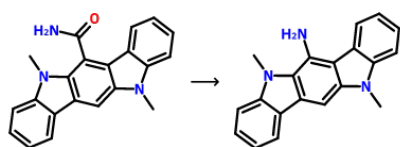


Reaction name: Hofmann rearrangement

Reaction conditions: KOH, Br₂, H₂O, 0 deg C or NaOCl, NaOH, H₂O, from 0 deg C to 75 deg C

Solvent: H₂O

Literature reference: 10.1016/S0022-1139(97)00097-3 and 10.1021/jm000950v and 10.1016/j.bmcl.2012.01.047 (Supporting Information S12) and 10.1002/chem.200390079 and 10.1021/cr040679f (large-scale application)

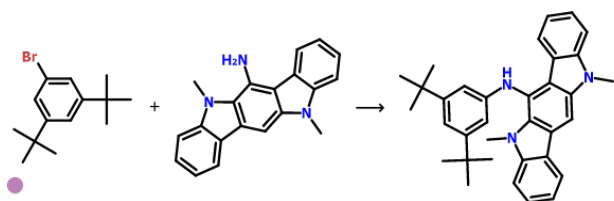


Reaction name: Buchwald-Hartwig Amination with Aromatic Amines

Reaction conditions: [Pd]-catalyst, ligand, Cs₂CO₃, dioxane or [Pd]-catalyst, ligand, KOtBU, dioxane

Solvent: dioxane or toluene

Literature reference: DOI: 10.1021/jo991699y and 10.1002/anie.200601612 and 10.1038/s41586-018-0056-8 and 10.1021/acs.chemrev.6b00512 and 10.1021/op8000146



Path #4

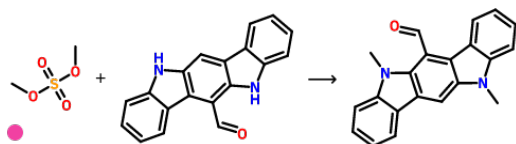
Score: 6.50 Estimated cost (\$/g): 399.62

Reaction name: N-heterocycle alkylation

Reaction conditions: KOH

Solvent: acetone

Literature reference: 10.1016/S0040-4020(98)00865-5

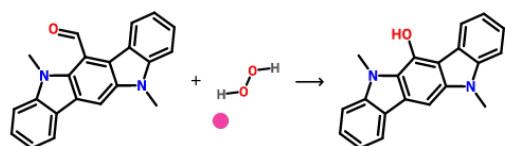


Reaction name: Dakin oxidation

Reaction conditions: UHP, NaOH, MeOH, 0 deg C

Solvent: MeOH

Literature reference: 10.1002/9780470638859.conrr175 ; 10.1021/op400101p

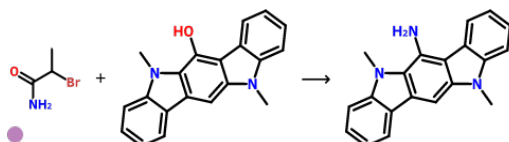


Reaction name: Smiles rearrangement

Reaction conditions: DMSO, KOH then KOH, heating

Solvent: DMSO

Literature reference: 10.1055/s-0033-1338703

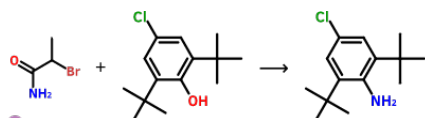


Reaction name: Smiles rearrangement

Reaction conditions: DMSO, KOH then KOH, heating

Solvent: DMSO

Literature reference: 10.1055/s-0033-1338703



Reaction name: Reductive decomposition of diazonium salts

Reaction conditions: NaNO₂, HCl, water, 0-5 deg C then H₃PO₂, hexane, water, rt

Solvent: water

Literature reference: EP0929544 (7.B Step B) and US4053527 (Example 1) and 10.1080/00397910802499542

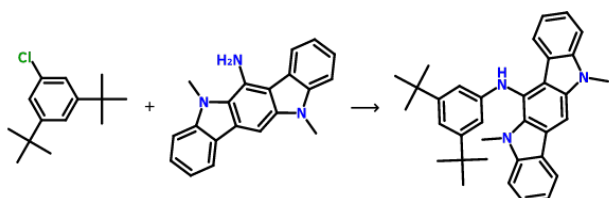


Reaction name: Buchwald-Hartwig Amination with Aromatic Amines

Reaction conditions: [Pd]-catalyst, ligand, Cs₂CO₃, dioxane or [Pd]-catalyst, ligand, KOtBU, dioxane

Solvent: dioxane or toluene

Literature reference: 10.1021/ja077074w and 10.1002/ejoc.201403428 and 10.1002/adsc.200700328 and 10.1021/op8000146



Path #5

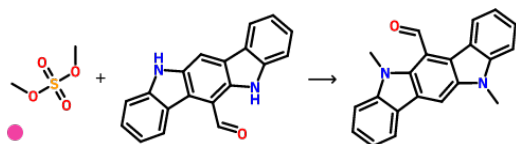
Score: 6.50 Estimated cost (\$/g): 117.12

Reaction name: N-heterocycle alkylation

Reaction conditions: KOH

Solvent: acetone

Literature reference: 10.1016/S0040-4020(98)00865-5

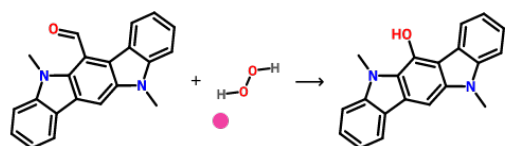


Reaction name: Dakin oxidation

Reaction conditions: UHP, NaOH, MeOH, 0 deg C

Solvent: MeOH

Literature reference: 10.1002/9780470638859.conrr175 ; 10.1021/op400101p

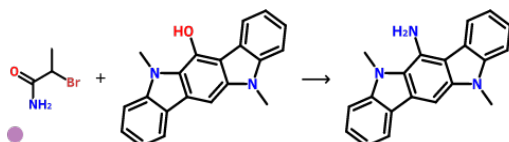


Reaction name: Smiles rearrangement

Reaction conditions: DMSO, KOH then KOH, heating

Solvent: DMSO

Literature reference: 10.1055/s-0033-1338703



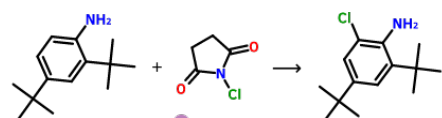
Reaction name: Electrophilic aromatic chlorination

Reaction conditions: NCS

Solvent: DCM or DMF

Alternative Solvent: DMSO

Literature reference: 10.1016/j.ejmech.2017.02.063 and 10.1002/adsc.200303229



Reaction name: Reductive decomposition of diazonium salts

Reaction conditions: NaNO₂, HCl, water, 0-5 deg C then H₃PO₂, hexane, water, rt

Solvent: water

Literature reference: EP0929544 (7.B Step B) and US4053527 (Example 1) and 10.1080/00397910802499542

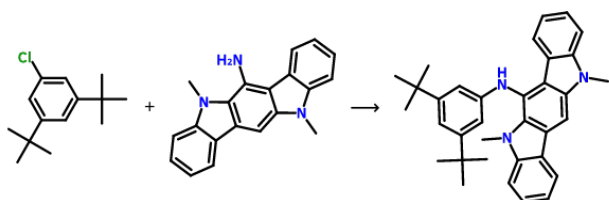


Reaction name: Buchwald-Hartwig Amination with Aromatic Amines

Reaction conditions: [Pd]-catalyst, ligand, Cs₂CO₃, dioxane or [Pd]-catalyst, ligand, KOtBU, dioxane

Solvent: dioxane or toluene

Literature reference: 10.1021/ja077074w and 10.1002/ejoc.201403428 and 10.1002/adsc.200700328 and 10.1021/op8000146



Path #6

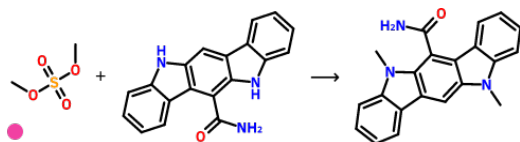
Score: 7.00 Estimated cost (\$/g): 1093.16

Reaction name: N-heterocycle alkylation

Reaction conditions: KOH

Solvent: acetone

Literature reference: 10.1016/S0040-4020(98)00865-5

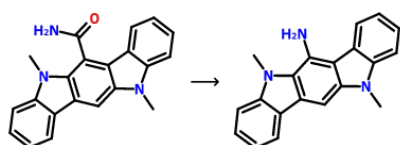


Reaction name: Hofmann rearrangement

Reaction conditions: KOH, Br₂, H₂O, 0 deg C or NaOCl, NaOH, H₂O, from 0 deg C to 75 deg C

Solvent: H₂O

Literature reference: 10.1016/S0022-1139(97)00097-3 and 10.1021/jm000950v and 10.1016/j.bmcl.2012.01.047 (Supporting Information S12) and 10.1002/chem.200390079 and 10.1021/cr040679f (large-scale application)

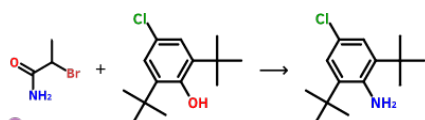


Reaction name: Smiles rearrangement

Reaction conditions: DMSO, KOH then KOH, heating

Solvent: DMSO

Literature reference: 10.1055/s-0033-1338703

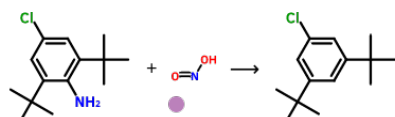


Reaction name: Reductive decomposition of diazonium salts

Reaction conditions: NaNO₂, HCl, water, 0-5 deg C then H₃PO₂, hexane, water, rt

Solvent: water

Literature reference: EP0929544 (7.B Step B) and US4053527 (Example 1) and 10.1080/00397910802499542

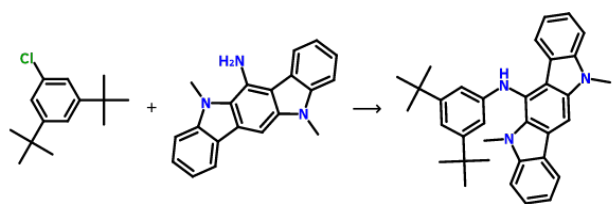


Reaction name: Buchwald-Hartwig Amination with Aromatic Amines

Reaction conditions: [Pd]-catalyst, ligand, Cs₂CO₃, dioxane or [Pd]-catalyst, ligand, KOtBU, dioxane

Solvent: dioxane or toluene

Literature reference: 10.1021/ja077074w and 10.1002/ejoc.201403428 and 10.1002/adsc.200700328 and 10.1021/op8000146



Path #7

Score: 8.00 Estimated cost (\$/g): 744.90

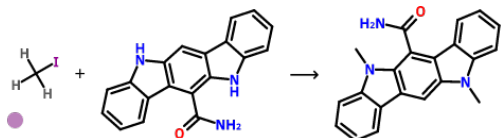
Reaction name: N-heterocycle alkylation

Reaction conditions: K₂CO₃

Solvent: DMF

Alternative Solvent: DMSO

Literature reference: 10.1039/C2OB26456K and 10.1016/j.bmc.2013.12.031

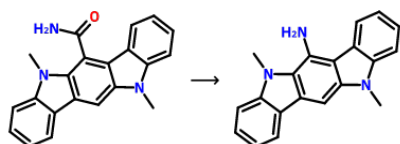


Reaction name: Hofmann rearrangement

Reaction conditions: KOH, Br₂, H₂O, 0 deg C or NaOCl, NaOH, H₂O, from 0 deg C to 75 deg C

Solvent: H₂O

Literature reference: 10.1016/S0022-1139(97)00097-3 and 10.1021/jm000950v and 10.1016/j.bmcl.2012.01.047 (Supporting Information S12) and 10.1002/chem.200390079 and 10.1021/cr040679f (large-scale application)

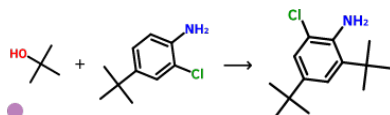


Reaction name: Friedel-Crafts alkylation with tertiary alcohol

Reaction conditions: H₂SO₄ or AlCl₃ or BF₃·Et₂O

Solvent: DCM

Literature reference: 10.1002/ejoc.201000070 and 10.1002/chem.201203042 (SI p.4) and 10.1021/jo01348a005



Reaction name: Reductive decomposition of diazonium salts

Reaction conditions: NaNO₂, HCl, water, 0-5 deg C then H₃PO₂, hexane, water, rt

Solvent: water

Literature reference: EP0929544 (7.B Step B) and US4053527 (Example 1) and 10.1080/00397910802499542

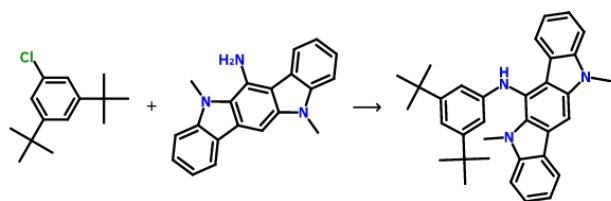


Reaction name: Buchwald-Hartwig Amination with Aromatic Amines

Reaction conditions: [Pd]-catalyst, ligand, Cs₂CO₃, dioxane or [Pd]-catalyst, ligand, KOtBU, dioxane

Solvent: dioxane or toluene

Literature reference: 10.1021/ja077074w and 10.1002/ejoc.201403428 and 10.1002/adsc.200700328 and 10.1021/op8000146



Path #8

Score: 11.00 Estimated cost (\$/g): 978.94

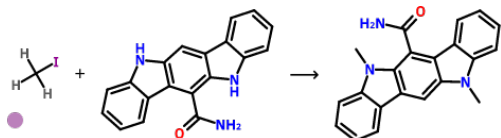
Reaction name: N-heterocycle alkylation

Reaction conditions: K₂CO₃

Solvent: DMF

Alternative Solvent: DMSO

Literature reference: 10.1039/C2OB26456K and 10.1016/j.bmc.2013.12.031

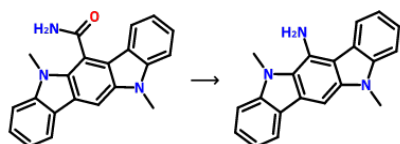


Reaction name: Hofmann rearrangement

Reaction conditions: KOH, Br₂, H₂O, 0 deg C or NaOCl, NaOH, H₂O, from 0 deg C to 75 deg C

Solvent: H₂O

Literature reference: 10.1016/S0022-1139(97)00097-3 and 10.1021/jm000950v and 10.1016/j.bmcl.2012.01.047 (Supporting Information S12) and 10.1002/chem.200390079 and 10.1021/cr040679f (large-scale application)

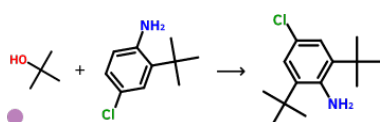


Reaction name: Friedel-Crafts alkylation with tertiary alcohol

Reaction conditions: H₂SO₄ or AlCl₃ or BF₃·Et₂O

Solvent: DCM

Literature reference: 10.1002/ejoc.201000070 and 10.1002/chem.201203042 (SI p.4) and 10.1021/jo01348a005



Reaction name: Reductive decomposition of diazonium salts

Reaction conditions: NaNO₂, HCl, water, 0-5 deg C then H₃PO₂, hexane, water, rt

Solvent: water

Literature reference: EP0929544 (7.B Step B) and US4053527 (Example 1) and 10.1080/00397910802499542

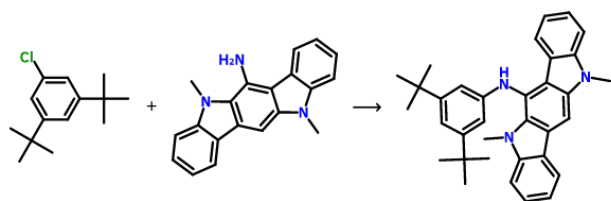


Reaction name: Buchwald-Hartwig Amination with Aromatic Amines

Reaction conditions: [Pd]-catalyst, ligand, Cs₂CO₃, dioxane or [Pd]-catalyst, ligand, KOtBU, dioxane

Solvent: dioxane or toluene

Literature reference: 10.1021/ja077074w and 10.1002/ejoc.201403428 and 10.1002/adsc.200700328 and 10.1021/op8000146



Path #9

Score: 12.00 Estimated cost (\$/g): 810.79

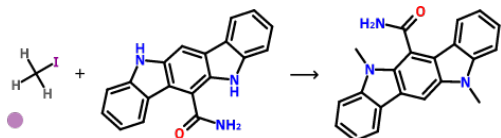
Reaction name: N-heterocycle alkylation

Reaction conditions: K₂CO₃

Solvent: DMF

Alternative Solvent: DMSO

Literature reference: 10.1039/C2OB26456K and 10.1016/j.bmc.2013.12.031

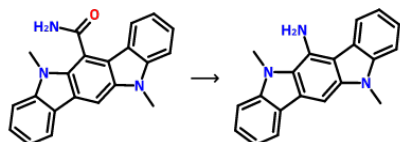


Reaction name: Hofmann rearrangement

Reaction conditions: KOH, Br₂, H₂O, 0 deg C or NaOCl, NaOH, H₂O, from 0 deg C to 75 deg C

Solvent: H₂O

Literature reference: 10.1016/S0022-1139(97)00097-3 and 10.1021/jm000950v and 10.1016/j.bmcl.2012.01.047 (Supporting Information S12) and 10.1002/chem.200390079 and 10.1021/cr040679f (large-scale application)



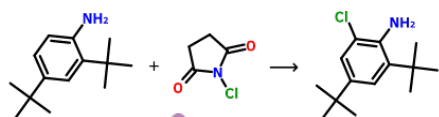
Reaction name: Electrophilic aromatic chlorination

Reaction conditions: NCS

Solvent: DCM or DMF

Alternative Solvent: DMSO

Literature reference: 10.1016/j.ejmech.2017.02.063 and 10.1002/adsc.200303229

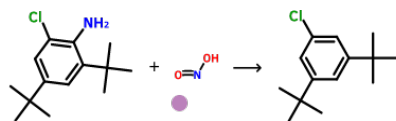


Reaction name: Reductive decomposition of diazonium salts

Reaction conditions: NaNO₂, HCl, water, 0-5 deg C then H₃PO₂, hexane, water, rt

Solvent: water

Literature reference: EP0929544 (7.B Step B) and US4053527 (Example 1) and 10.1080/00397910802499542

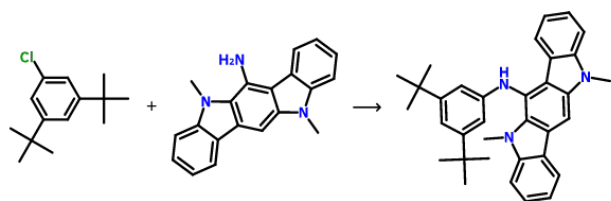


Reaction name: Buchwald-Hartwig Amination with Aromatic Amines

Reaction conditions: [Pd]-catalyst, ligand, Cs₂CO₃, dioxane or [Pd]-catalyst, ligand, KOtBU, dioxane

Solvent: dioxane or toluene

Literature reference: 10.1021/ja077074w and 10.1002/ejoc.201403428 and 10.1002/adsc.200700328 and 10.1021/op8000146



Path #10

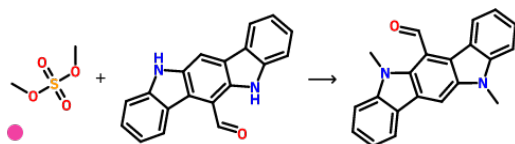
Score: 15.00 Estimated cost (\$/g): 51.23

Reaction name: N-heterocycle alkylation

Reaction conditions: KOH

Solvent: acetone

Literature reference: 10.1016/S0040-4020(98)00865-5

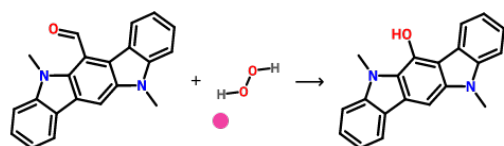


Reaction name: Dakin oxidation

Reaction conditions: UHP, NaOH, MeOH, 0 deg C

Solvent: MeOH

Literature reference: 10.1002/9780470638859.conrr175 ; 10.1021/op400101p

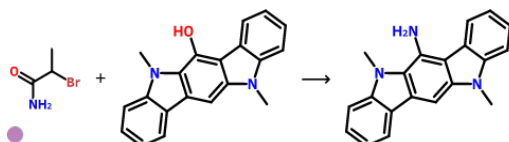


Reaction name: Smiles rearrangement

Reaction conditions: DMSO, KOH then KOH, heating

Solvent: DMSO

Literature reference: 10.1055/s-0033-1338703

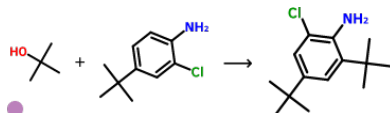


Reaction name: Friedel-Crafts alkylation with tertiary alcohol

Reaction conditions: H2SO4 or AlCl3 or BF3*Et2O

Solvent: DCM

Literature reference: 10.1002/ejoc.201000070 and 10.1002/chem.201203042 (SI p.4) and 10.1021/jo01348a005

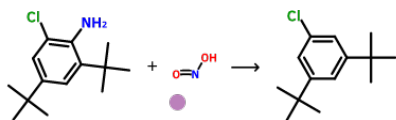


Reaction name: Reductive decomposition of diazonium salts

Reaction conditions: NaNO2, HCl, water, 0-5 deg C then H3PO2, hexane, water, rt

Solvent: water

Literature reference: EP0929544 (7.B Step B) and US4053527 (Example 1) and 10.1080/00397910802499542



Reaction name: Buchwald-Hartwig Amination with Aromatic Amines

Reaction conditions: [Pd]-catalyst, ligand, Cs₂CO₃, dioxane or [Pd]-catalyst, ligand, KOtBU, dioxane

Solvent: dioxane or toluene

Literature reference: 10.1021/ja077074w and 10.1002/ejoc.201403428 and 10.1002/adsc.200700328 and 10.1021/op8000146

