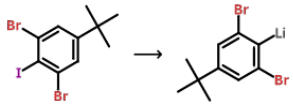
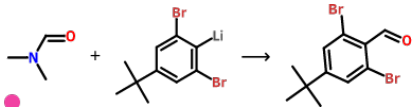
Path #1

Score: 5.00 Estimated cost ($/g): 94.56

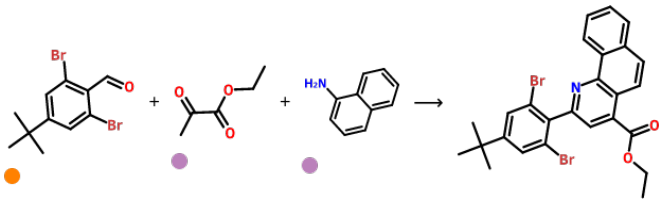
Reaction name: Synthesis of organolithium reagents
Reaction conditions: Li, Et2O or Li, THF
Solvent: Et2O or THF
Alternative Solvent: t-Butyl ethyl ether
Literature reference: 10.1002/cmdc.201600408 and 10.1002/1521-3773(20020503)41%3A9<1610%3A%3AAID-ANIE1610>3.0.CO%3B2-T



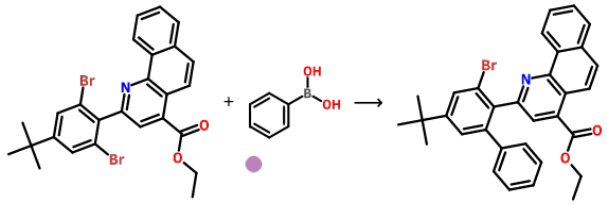
Reaction name: Formylation of organolithium reagents
Reaction conditions: THF, -78 deg C
Solvent: THF
Alternative Solvent: t-Butyl ethyl ether
Literature reference: 10.1021/jm950639r and 10.1016/S0040-4039(00)78337-7 and 10.24820/ark.5550190.p011.464



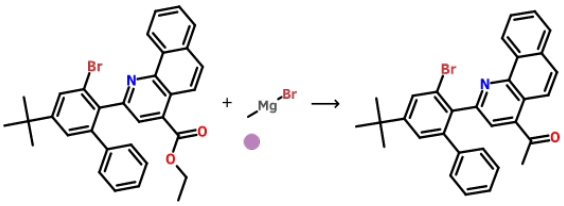
Reaction name: Doebner reaction
Reaction conditions: FeCl3 or I2
Solvent: EtOH
Literature reference: 10.1039/D0GC00738B and 10.3184/174751911X13148095775284 and 10.1016/j.bioorg.2020.104373 and 10.1002/jhet.3730 and 10.1016/j.jfluchem.2009.01.002 and 10.1055/s-2008-1067087



Reaction name: Suzuki Aryl-Aryl Coupling
Reaction conditions: [Pd]-catalyst, ligand, base
Solvent: dioxane
Alternative Solvent: CPME
Literature reference: 10.1126/science.aaa5414 and 10.1021/cr100346g



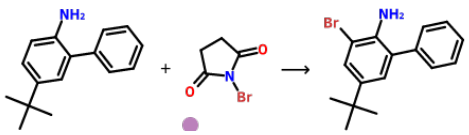
Reaction name: Addition of organometallic reagents to esters
Reaction conditions: morpholine, DiBAL-H, THF, -78 deg C to rt
Solvent: THF
Alternative Solvent: t-Butyl ethyl ether
Literature reference: 10.1016/j.tet.2014.03.045



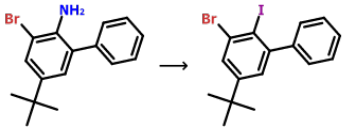
Path #2

Score: 6.00 Estimated cost ($/g): 13.51

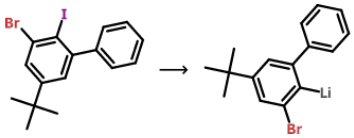
Reaction name: Electrophilic aromatic bromination
Reaction conditions: NBS
Solvent: DCM or DMF
Alternative Solvent: DMSO
Literature reference: 10.1016/j.tetlet.2003.08.069 and 10.1016/j.ejmech.2017.06.006



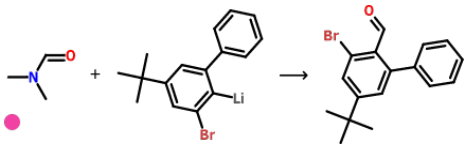
Reaction name: Sandmeyer reaction
Reaction conditions: ispentyl nitirite, diiodomethane, CuI
Solvent: THF or MeCN
Literature reference: 10.1021/jm010952v and 10.1021/jo00295a056



Reaction name: Synthesis of organolithium reagents
Reaction conditions: Li, Et2O or Li, THF
Solvent: Et2O or THF
Alternative Solvent: t-Butyl ethyl ether
Literature reference: 10.1002/cmdc.201600408 and 10.1002/1521-3773(20020503)41%3A9<1610%3A%3AAID-ANIE1610>3.0.CO%3B2-T

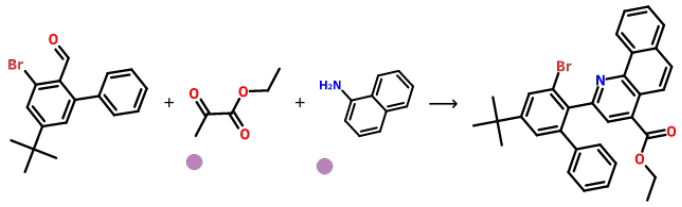


Reaction name: Formylation of organolithium reagents
Reaction conditions: THF, -78 deg C
Solvent: THF
Alternative Solvent: t-Butyl ethyl ether
Literature reference: 10.1021/jm950639r and 10.1016/S0040-4039(00)78337-7 and 10.24820/ark.5550190.p011.464

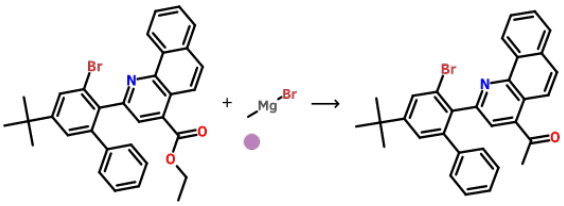


Reaction name: Doebner reaction
Reaction conditions: FeCl3 or I2
Solvent: EtOH
Literature reference: 10.1039/D0GC00738B and 10.3184/174751911X13148095775284 and

10.1016/j.bioorg.2020.104373 and 10.1002/jhet.3730 and 10.1016/j.jfluchem.2009.01.002 and 10.1055/s-2008-1067087



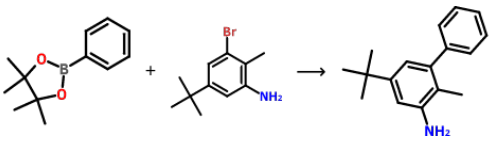
Reaction name: Addition of organometallic reagents to esters
Reaction conditions: morpholine, DiBAL-H, THF, -78 deg C to rt
Solvent: THF
Alternative Solvent: t-Butyl ethyl ether
Literature reference: 10.1016/j.tet.2014.03.045



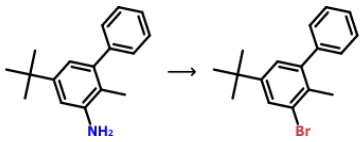
Path #3

Score: 6.50 Estimated cost ($/g): 344.55

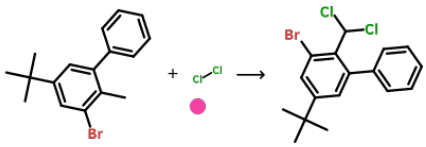
Reaction name: Suzuki Aryl-Aryl Coupling
Reaction conditions: [Pd]-catalyst, ligand, base
Solvent: dioxane
Alternative Solvent: CPME
Literature reference: 10.1126/science.aaa5414 and 10.1021/cr100346g



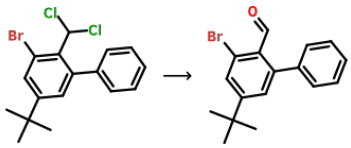
Reaction name: Sandmeyer reaction
Reaction conditions: HBr, NaNO2, CuBr
Solvent: THF or MeCN
Literature reference: 10.1021/ja034563x and 10.1016/j.jfluchem.2007.07.011 and 10.1016/j.tet.2013.02.016



Reaction name: Dichlorination of methylarenes
Reaction conditions: Cl2, hv
Solvent: CCl4 or benzene or THF
Alternative Solvent: Fluorobenzene or t-Butyl ethyl ether
Literature reference: 10.1021/ja00061a002 and 10.1021/jo00241a031

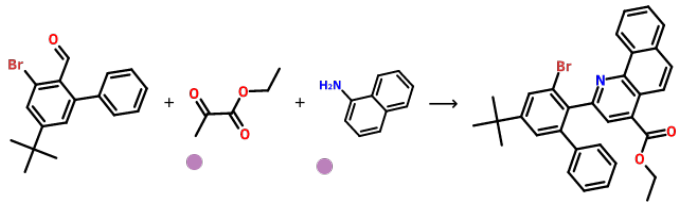


Reaction name: Hydrolysis of dichloromethyl group
Reaction conditions: AcONa, EtOH, H2O, heat
Solvent: H2O or EtOH
Literature reference: 10.1016/j.bmcl.2009.09.056 and 10.1055/s-2002-35990 and 10.1002/jhet.5570290403

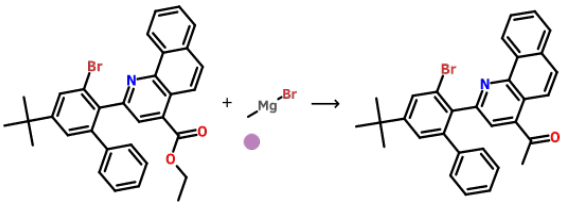


Reaction name: Doebner reaction
Reaction conditions: FeCl3 or I2
Solvent: EtOH
Literature reference: 10.1039/D0GC00738B and 10.3184/174751911X13148095775284 and

10.1016/j.bioorg.2020.104373 and 10.1002/jhet.3730 and 10.1016/j.jfluchem.2009.01.002 and 10.1055/s-2008-1067087



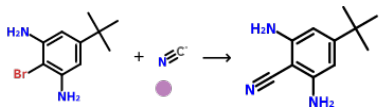
Reaction name: Addition of organometallic reagents to esters
Reaction conditions: morpholine, DiBAL-H, THF, -78 deg C to rt
Solvent: THF
Alternative Solvent: t-Butyl ethyl ether
Literature reference: 10.1016/j.tet.2014.03.045



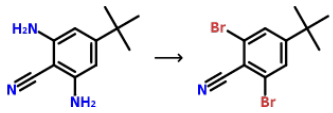
Path #4

Score: 6.50 Estimated cost ($/g): 249.59

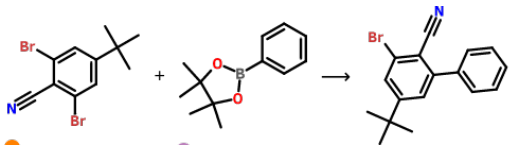
Reaction name: Cyanation of aryl halides
Reaction conditions: CuCN, DMF, 80-150 deg C or K4[Fe(CN)6], Pd(OAc)2, iPrOH, H2O, NMP, 140 deg C
Solvent: NMP
Alternative Solvent: formamide
Literature reference: 10.1021/op034110c (industrial application) and 10.1021/op200326s (industrial application) and 10.1021/op9000725 (industrial application)



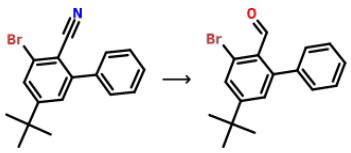
Reaction name: Sandmeyer reaction
Reaction conditions: HBr, NaNO2, CuBr
Solvent: THF or MeCN
Literature reference: 10.1021/ja034563x and 10.1016/j.jfluchem.2007.07.011 and 10.1016/j.tet.2013.02.016



Reaction name: Suzuki Aryl-Aryl Coupling
Reaction conditions: [Pd]-catalyst, ligand, base
Solvent: dioxane
Alternative Solvent: CPME
Literature reference: 10.1126/science.aaa5414 and 10.1021/cr100346g

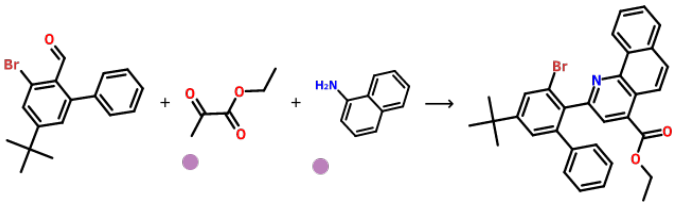


Reaction name: Reduction of nitriles to aldehydes
Reaction conditions: DIBAL, toluene
Solvent: toluene or DCM or THF or hexane
Literature reference: 10.1002/anie.200704095 and 10.1002/ejoc.200390130

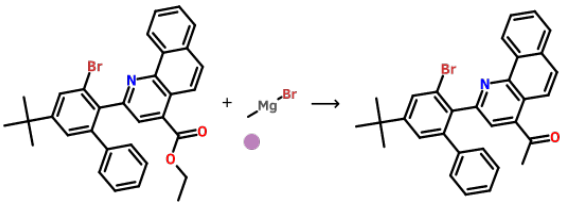


Reaction name: Doebner reaction
Reaction conditions: FeCl3 or I2
Solvent: EtOH
Literature reference: 10.1039/D0GC00738B and 10.3184/174751911X13148095775284 and 10.1016/j.bioorg.2020.104373 and 10.1002/jhet.3730 and 10.1016/j.jfluchem.2009.01.002 and

10.1055/s-2008-1067087



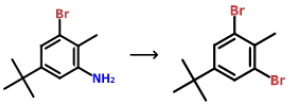
Reaction name: Addition of organometallic reagents to esters
Reaction conditions: morpholine, DiBAL-H, THF, -78 deg C to rt
Solvent: THF
Alternative Solvent: t-Butyl ethyl ether
Literature reference: 10.1016/j.tet.2014.03.045



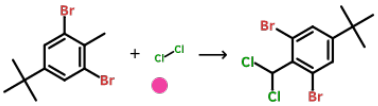
Path #5

Score: 6.50 Estimated cost ($/g): 344.55

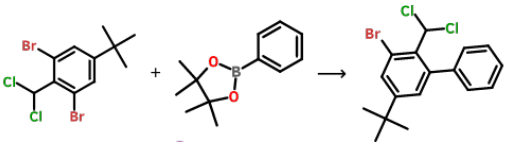
Reaction name: Sandmeyer reaction
Reaction conditions: HBr, NaNO2, CuBr
Solvent: THF or MeCN
Literature reference: 10.1021/ja034563x and 10.1016/j.jfluchem.2007.07.011 and 10.1016/j.tet.2013.02.016



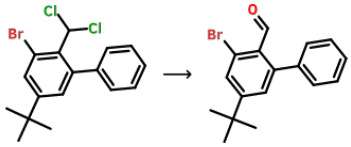
Reaction name: Dichlorination of methylarenes
Reaction conditions: Cl2, hv
Solvent: CCl4 or benzene or THF
Alternative Solvent: Fluorobenzene or t-Butyl ethyl ether
Literature reference: 10.1021/ja00061a002 and 10.1021/jo00241a031



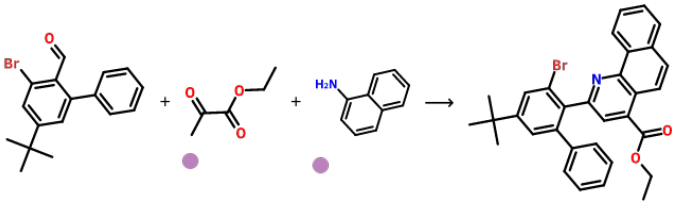
Reaction name: Suzuki Aryl-Aryl Coupling
Reaction conditions: [Pd]-catalyst, ligand, base
Solvent: dioxane
Alternative Solvent: CPME
Literature reference: 10.1126/science.aaa5414 and 10.1021/cr100346g



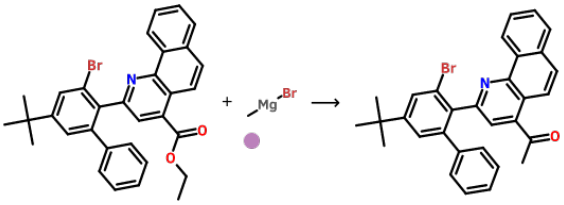
Reaction name: Hydrolysis of dichloromethyl group
Reaction conditions: AcONa, EtOH, H2O, heat
Solvent: H2O or EtOH
Literature reference: 10.1016/j.bmcl.2009.09.056 and 10.1055/s-2002-35990 and 10.1002/jhet.5570290403



Reaction name: Doebner reaction
Reaction conditions: FeCl3 or I2
Solvent: EtOH
Literature reference: 10.1039/D0GC00738B and 10.3184/174751911X13148095775284 and 10.1016/j.bioorg.2020.104373 and 10.1002/jhet.3730 and 10.1016/j.jfluchem.2009.01.002 and 10.1055/s-2008-1067087



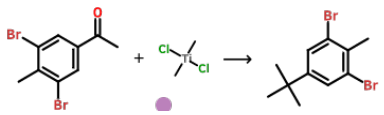
Reaction name: Addition of organometallic reagents to esters
Reaction conditions: morpholine, DiBAL-H, THF, -78 deg C to rt
Solvent: THF
Alternative Solvent: t-Butyl ethyl ether
Literature reference: 10.1016/j.tet.2014.03.045



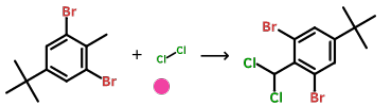
Path #6

Score: 6.50 Estimated cost ($/g): 504.12 missing prices for certain substrates, taking 10$/g

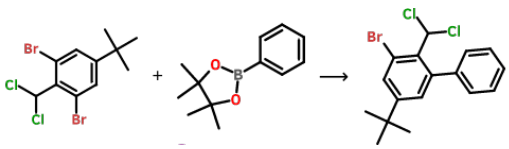
Reaction name: Gem-dimethylation of ketones
Reaction conditions: Me2TiCl2, DCM, -30 deg C
Solvent: DCM
Literature reference: 10.1039/C39810000237 and 10.1039/B924542A and 10.1002/anie.201003823



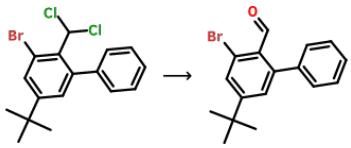
Reaction name: Dichlorination of methylarenes
Reaction conditions: Cl2, hv
Solvent: CCl4 or benzene or THF
Alternative Solvent: Fluorobenzene or t-Butyl ethyl ether
Literature reference: 10.1021/ja00061a002 and 10.1021/jo00241a031



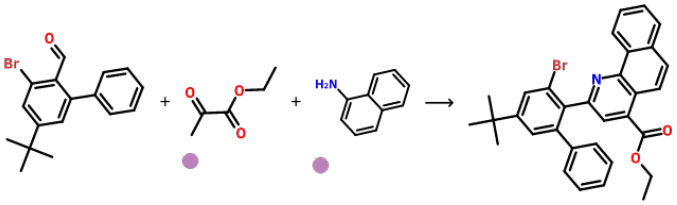
Reaction name: Suzuki Aryl-Aryl Coupling
Reaction conditions: [Pd]-catalyst, ligand, base
Solvent: dioxane
Alternative Solvent: CPME
Literature reference: 10.1126/science.aaa5414 and 10.1021/cr100346g



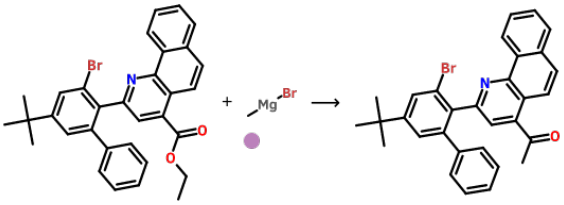
Reaction name: Hydrolysis of dichloromethyl group
Reaction conditions: AcONa, EtOH, H2O, heat
Solvent: H2O or EtOH
Literature reference: 10.1016/j.bmcl.2009.09.056 and 10.1055/s-2002-35990 and 10.1002/jhet.5570290403



Reaction name: Doebner reaction
Reaction conditions: FeCl3 or I2
Solvent: EtOH
Literature reference: 10.1039/D0GC00738B and 10.3184/174751911X13148095775284 and 10.1016/j.bioorg.2020.104373 and 10.1002/jhet.3730 and 10.1016/j.jfluchem.2009.01.002 and 10.1055/s-2008-1067087



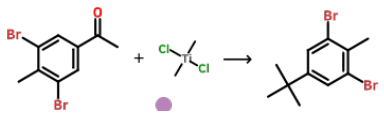
Reaction name: Addition of organometallic reagents to esters
Reaction conditions: morpholine, DiBAL-H, THF, -78 deg C to rt
Solvent: THF
Alternative Solvent: t-Butyl ethyl ether
Literature reference: 10.1016/j.tet.2014.03.045



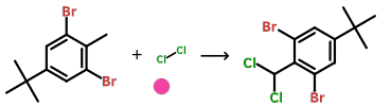
Path #7

Score: 7.00 Estimated cost ($/g): 504.12 missing prices for certain substrates, taking 10$/g

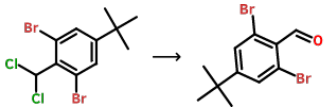
Reaction name: Gem-dimethylation of ketones
Reaction conditions: Me2TiCl2, DCM, -30 deg C
Solvent: DCM
Literature reference: 10.1039/C39810000237 and 10.1039/B924542A and 10.1002/anie.201003823



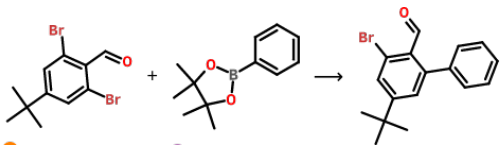
Reaction name: Dichlorination of methylarenes
Reaction conditions: Cl2, hv
Solvent: CCl4 or benzene or THF
Alternative Solvent: Fluorobenzene or t-Butyl ethyl ether
Literature reference: 10.1021/ja00061a002 and 10.1021/jo00241a031



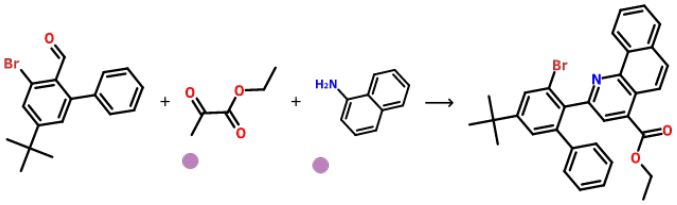
Reaction name: Hydrolysis of dichloromethyl group
Reaction conditions: AcONa, EtOH, H2O, heat
Solvent: H2O or EtOH
Literature reference: 10.1016/j.bmcl.2009.09.056 and 10.1055/s-2002-35990 and 10.1002/jhet.5570290403



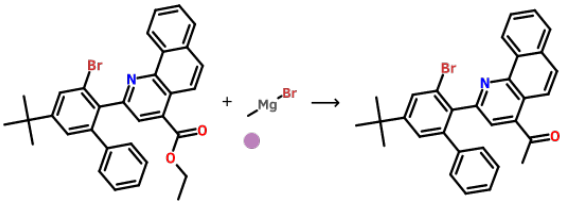
Reaction name: Suzuki Aryl-Aryl Coupling
Reaction conditions: [Pd]-catalyst, ligand, base
Solvent: dioxane
Alternative Solvent: CPME
Literature reference: 10.1126/science.aaa5414 and 10.1021/cr100346g



Reaction name: Doebner reaction
Reaction conditions: FeCl3 or I2
Solvent: EtOH
Literature reference: 10.1039/D0GC00738B and 10.3184/174751911X13148095775284 and 10.1016/j.bioorg.2020.104373 and 10.1002/jhet.3730 and 10.1016/j.jfluchem.2009.01.002 and 10.1055/s-2008-1067087



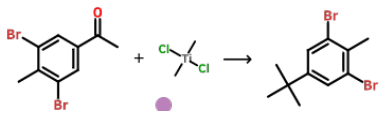
Reaction name: Addition of organometallic reagents to esters
Reaction conditions: morpholine, DiBAL-H, THF, -78 deg C to rt
Solvent: THF
Alternative Solvent: t-Butyl ethyl ether
Literature reference: 10.1016/j.tet.2014.03.045



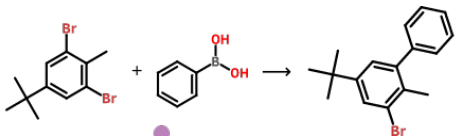
Path #8

Score: 7.00 Estimated cost ($/g): 503.18 missing prices for certain substrates, taking 10$/g

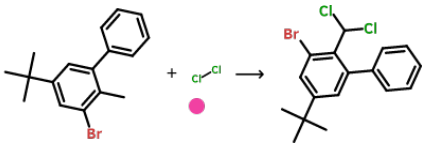
Reaction name: Gem-dimethylation of ketones
Reaction conditions: Me2TiCl2, DCM, -30 deg C
Solvent: DCM
Literature reference: 10.1039/C39810000237 and 10.1039/B924542A and 10.1002/anie.201003823



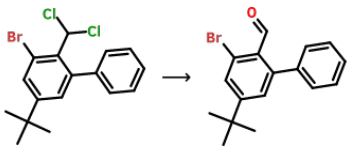
Reaction name: Suzuki Aryl-Aryl Coupling
Reaction conditions: [Pd]-catalyst, ligand, base
Solvent: dioxane
Alternative Solvent: CPME
Literature reference: 10.1126/science.aaa5414 and 10.1021/cr100346g



Reaction name: Dichlorination of methylarenes
Reaction conditions: Cl2, hv
Solvent: CCl4 or benzene or THF
Alternative Solvent: Fluorobenzene or t-Butyl ethyl ether
Literature reference: 10.1021/ja00061a002 and 10.1021/jo00241a031

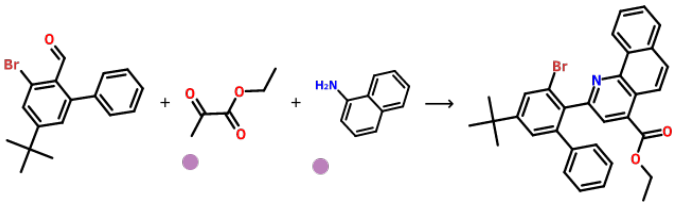


Reaction name: Hydrolysis of dichloromethyl group
Reaction conditions: AcONa, EtOH, H2O, heat
Solvent: H2O or EtOH
Literature reference: 10.1016/j.bmcl.2009.09.056 and 10.1055/s-2002-35990 and 10.1002/jhet.5570290403

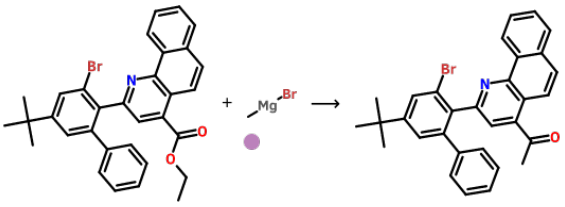


Reaction name: Doebner reaction
Reaction conditions: FeCl3 or I2
Solvent: EtOH
Literature reference: 10.1039/D0GC00738B and 10.3184/174751911X13148095775284 and 10.1016/j.bioorg.2020.104373 and 10.1002/jhet.3730 and 10.1016/j.jfluchem.2009.01.002 and

10.1055/s-2008-1067087



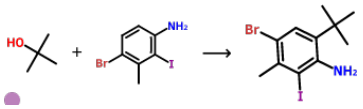
Reaction name: Addition of organometallic reagents to esters
Reaction conditions: morpholine, DiBAL-H, THF, -78 deg C to rt
Solvent: THF
Alternative Solvent: t-Butyl ethyl ether
Literature reference: 10.1016/j.tet.2014.03.045



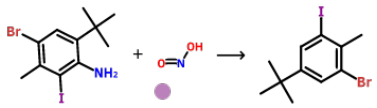
Path #9

Score: 7.50 Estimated cost ($/g): 319.71

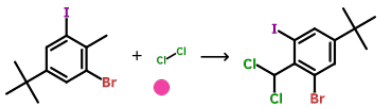
Reaction name: Friedel-Crafts alkylation with tertiary alcohol
Reaction conditions: H2SO4 or AlCl3 or BF3*Et2O
Solvent: DCM
Literature reference: 10.1002/ejoc.201000070 and 10.1002/chem.201203042 (SI p.4) and 10.1021/jo01348a005



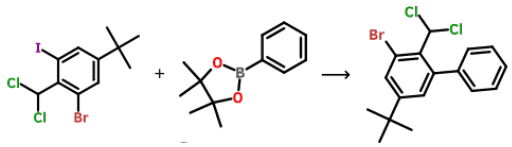
Reaction name: Reductive decomposition of diazonium salts
Reaction conditions: NaNO2, HCl, water, 0-5 deg C then H3PO2, hexane, water, rt
Solvent: water
Literature reference: EP0929544 (7.B Step B) and US4053527 (Example 1) and 10.1080/00397910802499542



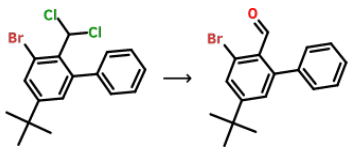
Reaction name: Dichlorination of methylarenes
Reaction conditions: Cl2, hv
Solvent: CCl4 or benzene or THF
Alternative Solvent: Fluorobenzene or t-Butyl ethyl ether
Literature reference: 10.1021/ja00061a002 and 10.1021/jo00241a031



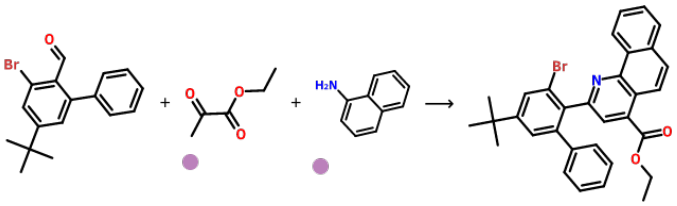
Reaction name: Suzuki Aryl-Aryl Coupling
Reaction conditions: [Pd]-catalyst, ligand, base
Solvent: dioxane
Alternative Solvent: CPME
Literature reference: 10.1126/science.aaa5414 and 10.1021/cr100346g



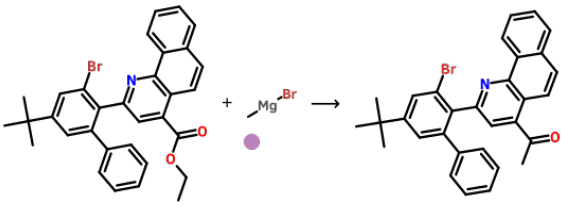
Reaction name: Hydrolysis of dichloromethyl group
Reaction conditions: AcONa, EtOH, H2O, heat
Solvent: H2O or EtOH
Literature reference: 10.1016/j.bmcl.2009.09.056 and 10.1055/s-2002-35990 and 10.1002/jhet.5570290403



Reaction name: Doebner reaction
Reaction conditions: FeCl3 or I2
Solvent: EtOH
Literature reference: 10.1039/D0GC00738B and 10.3184/174751911X13148095775284 and 10.1016/j.bioorg.2020.104373 and 10.1002/jhet.3730 and 10.1016/j.jfluchem.2009.01.002 and 10.1055/s-2008-1067087



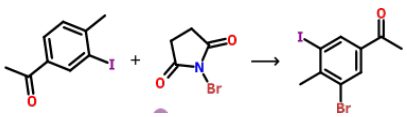
Reaction name: Addition of organometallic reagents to esters
Reaction conditions: morpholine, DiBAL-H, THF, -78 deg C to rt
Solvent: THF
Alternative Solvent: t-Butyl ethyl ether
Literature reference: 10.1016/j.tet.2014.03.045



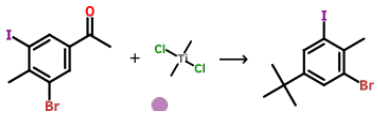
Path #10

Score: 7.50 Estimated cost ($/g): 143.79 missing prices for certain substrates, taking 10$/g

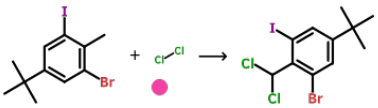
Reaction name: Electrophilic aromatic bromination
Reaction conditions: NBS
Solvent: DCM or DMF
Alternative Solvent: DMSO
Literature reference: 10.1016/j.tetlet.2003.08.069 and 10.1016/j.ejmech.2017.06.006



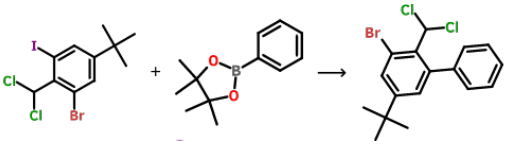
Reaction name: Gem-dimethylation of ketones
Reaction conditions: Me2TiCl2, DCM, -30 deg C
Solvent: DCM
Literature reference: 10.1039/C39810000237 and 10.1039/B924542A and 10.1002/anie.201003823



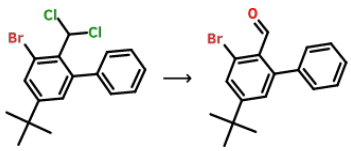
Reaction name: Dichlorination of methylarenes
Reaction conditions: Cl2, hv
Solvent: CCl4 or benzene or THF
Alternative Solvent: Fluorobenzene or t-Butyl ethyl ether
Literature reference: 10.1021/ja00061a002 and 10.1021/jo00241a031



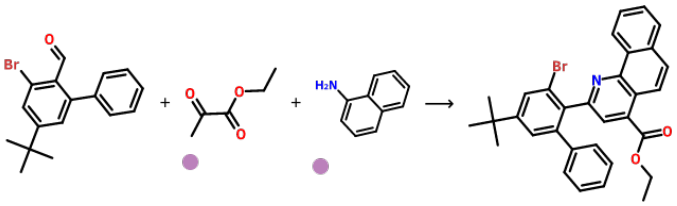
Reaction name: Suzuki Aryl-Aryl Coupling
Reaction conditions: [Pd]-catalyst, ligand, base
Solvent: dioxane
Alternative Solvent: CPME
Literature reference: 10.1126/science.aaa5414 and 10.1021/cr100346g



Reaction name: Hydrolysis of dichloromethyl group
Reaction conditions: AcONa, EtOH, H2O, heat
Solvent: H2O or EtOH
Literature reference: 10.1016/j.bmcl.2009.09.056 and 10.1055/s-2002-35990 and 10.1002/jhet.5570290403



Reaction name: Doebner reaction
Reaction conditions: FeCl3 or I2
Solvent: EtOH
Literature reference: 10.1039/D0GC00738B and 10.3184/174751911X13148095775284 and 10.1016/j.bioorg.2020.104373 and 10.1002/jhet.3730 and 10.1016/j.jfluchem.2009.01.002 and 10.1055/s-2008-1067087



Reaction name: Addition of organometallic reagents to esters
Reaction conditions: morpholine, DiBAL-H, THF, -78 deg C to rt
Solvent: THF
Alternative Solvent: t-Butyl ethyl ether
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