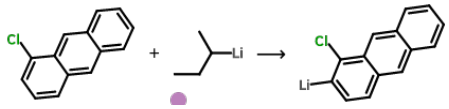
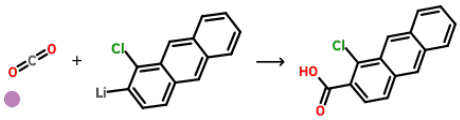
Path #1

Score: 7.00 Estimated cost ($/g): 210.49

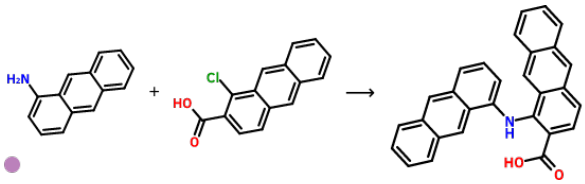
Reaction name: Directed ortho metalation
Reaction conditions: sBuLi, THF
Solvent: THF
Alternative Solvent: t-Butyl ethyl ether
Literature reference: 10.1016/j.tetlet.2004.01.122



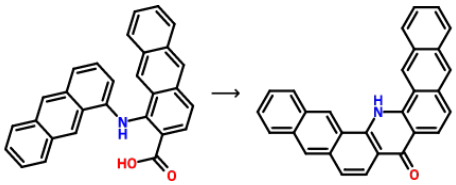
Reaction name: Carboxylation of organolithium reagents
Reaction conditions: THF, -78 deg C
Solvent: THF
Alternative Solvent: t-Butyl ethyl ether
Literature reference: 10.1016/S0040-4039(00)78337-7 and 10.1021/ja00308a025 and 10.1016/0040-4039(96)00415-7



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

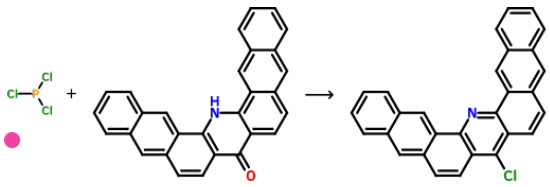


Reaction name: Formation of acridine
Reaction conditions: PPA
Solvent: none
Literature reference: 10.1055/s-1985-31164 (multigram-scale application)

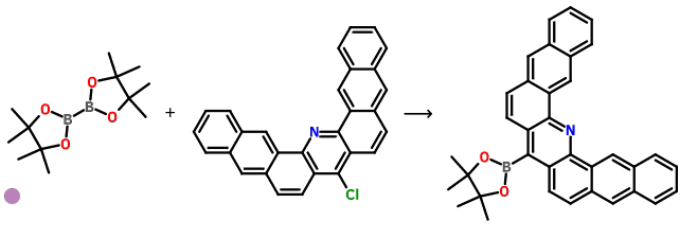


Reaction name: Nucleophilic aromatic chlorination
Reaction conditions: PCl3, DMF

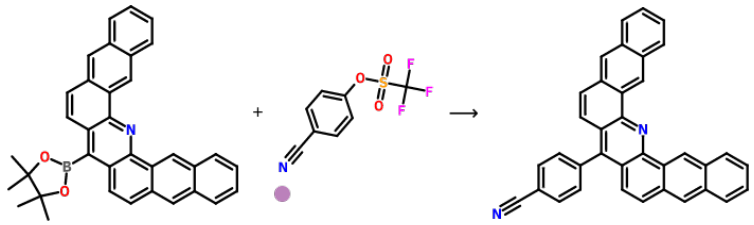
Solvent: DMF
Alternative Solvent: DMSO
Literature reference: 10.1021/jm051146h and 10.1016/j.bmc.2013.06.026 and 10.1016/j.ejmech.2010.05.030



Reaction name: Coupling of B2(pin)2 with aryl halide
Reaction conditions: Pd-cat, AcOK, 1,4-dioxane, 70-110 deg C
Solvent: dioxane or THF or DMF or toluene or DMSO
Literature reference: 10.1021/ol0171463 and 10.1021/jo202472k and 10.1021/jm051065l and 10.1021/acs.oprd.2c00057 (industrial application)



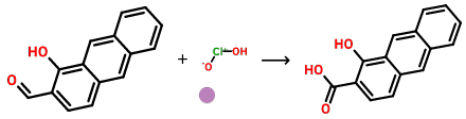
Reaction name: Suzuki Aryl-Aryl Coupling
Reaction conditions: [Pd]-catalyst, ligand, base
Solvent: dioxane
Alternative Solvent: CPME
Literature reference: 10.1126/science.aaa5414 and 10.1021/cr100346g



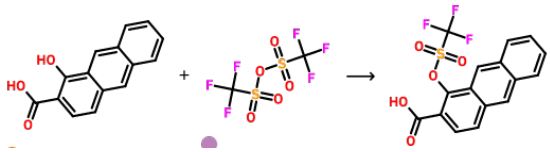
Path #2

Score: 11.50 Estimated cost ($/g): 591.54

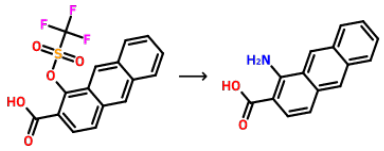
Reaction name: Pinnick oxidation
Reaction conditions: NaClO2, tBuOH, NaH2PO4, 2-methyl-2-butene
Solvent: water
Literature reference: 10.1021/ol401115a and 10.1055/s-2006-942426 and 10.1021/cr040679f (large-scale application)



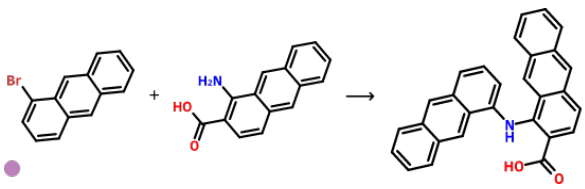
Reaction name: O-sulfonylation
Reaction conditions: NEt3
Solvent: DCM or toluene
Literature reference: 10.1016/j.bmcl.2011.02.024 and 10.1055/s-1998-2113 (experimental)



Reaction name: Buchwald Hartwig Amination
Reaction conditions: NH3, Pd[(o-tol)3P]2, NaOtBu, CyPF-t-Bu, dioxane
Solvent: dioxane
Alternative Solvent: CPME
Literature reference: 10.1021/ja903049z and 10.1021/ol401612c and 10.1021/ol501739g and 10.1021/op8000146 and WO2008133459 (Preparation Examples 9-14) and EP2149555 (Synthesis Example 7)

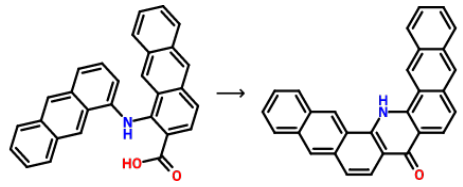


Reaction name: Buchwald-Hartwig Amination with Aromatic Amines
Reaction conditions: [Pd]-catalyst, ligand, Cs2CO3, dioxane or [Pd]-catalyst, ligand, KOtBU, dioxane
Solvent: dioxane or toluene
Literature reference: DOI: 10.1021/jo991699y and 10.1002/anie.200601612 and 10.1038/s41586-018-0056-8 and 10.1021/acs.chemrev.6b00512 and 10.1021/op8000146

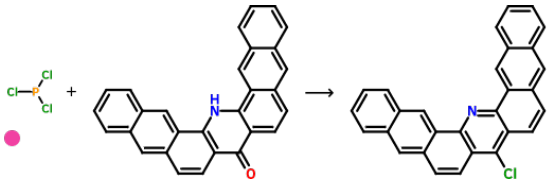


Reaction name: Formation of acridine

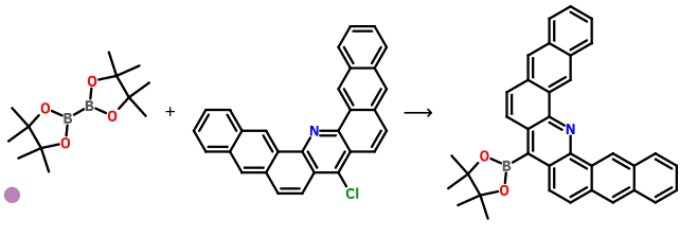
Reaction conditions: PPA
Solvent: none
Literature reference: 10.1055/s-1985-31164 (multigram-scale application)



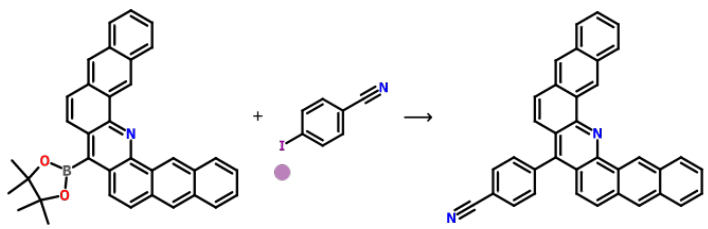
Reaction name: Nucleophilic aromatic chlorination
Reaction conditions: PCl3, DMF
Solvent: DMF
Alternative Solvent: DMSO
Literature reference: 10.1021/jm051146h and 10.1016/j.bmc.2013.06.026 and 10.1016/j.ejmech.2010.05.030



Reaction name: Coupling of B2(pin)2 with aryl halide
Reaction conditions: Pd-cat, AcOK, 1,4-dioxane, 70-110 deg C
Solvent: dioxane or THF or DMF or toluene or DMSO
Literature reference: 10.1021/ol0171463 and 10.1021/jo202472k and 10.1021/jm051065l and 10.1021/acs.oprd.2c00057 (industrial application)



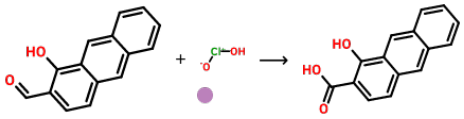
Reaction name: Suzuki Aryl-Aryl Coupling
Reaction conditions: [Pd]-catalyst, ligand, base
Solvent: dioxane
Alternative Solvent: CPME
Literature reference: 10.1126/science.aaa5414 and 10.1021/cr100346g



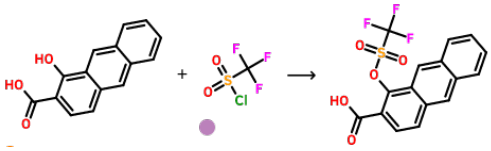
Path #3

Score: 11.50 Estimated cost ($/g): 583.70

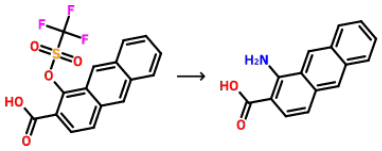
Reaction name: Pinnick oxidation
Reaction conditions: NaClO2, tBuOH, NaH2PO4, 2-methyl-2-butene
Solvent: water
Literature reference: 10.1021/ol401115a and 10.1055/s-2006-942426 and 10.1021/cr040679f (large-scale application)



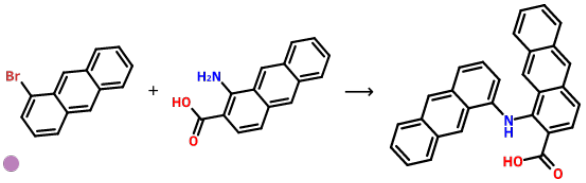
Reaction name: O-sulfonylation
Reaction conditions: NEt3
Solvent: DCM or THF
Alternative Solvent: t-Butyl ethyl ether
Literature reference: 10.1081/SCC-120030306 and 10.1002/ejoc.200900067 (experimental)



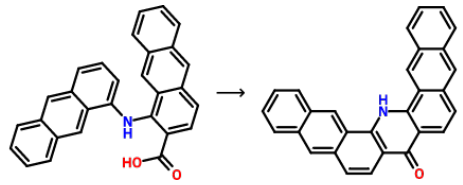
Reaction name: Buchwald Hartwig Amination
Reaction conditions: NH3, Pd[(o-tol)3P]2, NaOtBu, CyPF-t-Bu, dioxane
Solvent: dioxane
Alternative Solvent: CPME
Literature reference: 10.1021/ja903049z and 10.1021/ol401612c and 10.1021/ol501739g and 10.1021/op8000146 and WO2008133459 (Preparation Examples 9-14) and EP2149555 (Synthesis Example 7)



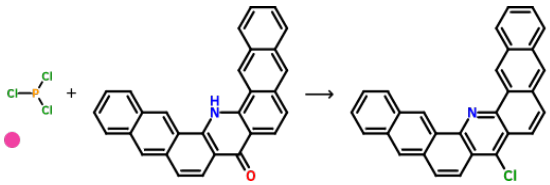
Reaction name: Buchwald-Hartwig Amination with Aromatic Amines
Reaction conditions: [Pd]-catalyst, ligand, Cs2CO3, dioxane or [Pd]-catalyst, ligand, KOtBU, dioxane
Solvent: dioxane or toluene
Literature reference: DOI: 10.1021/jo991699y and 10.1002/anie.200601612 and 10.1038/s41586-018-0056-8 and 10.1021/acs.chemrev.6b00512 and 10.1021/op8000146



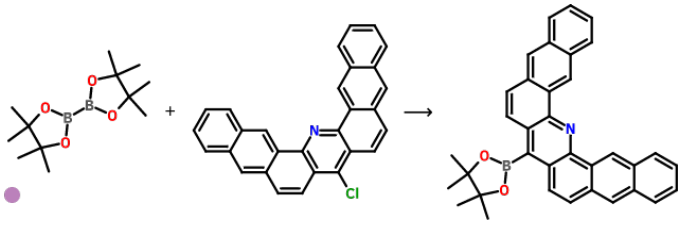
Reaction name: Formation of acridine
Reaction conditions: PPA
Solvent: none
Literature reference: 10.1055/s-1985-31164 (multigram-scale application)



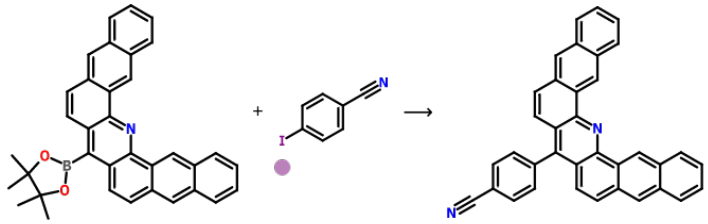
Reaction name: Nucleophilic aromatic chlorination
Reaction conditions: PCl3, DMF
Solvent: DMF
Alternative Solvent: DMSO
Literature reference: 10.1021/jm051146h and 10.1016/j.bmc.2013.06.026 and 10.1016/j.ejmech.2010.05.030



Reaction name: Coupling of B2(pin)2 with aryl halide
Reaction conditions: Pd-cat, AcOK, 1,4-dioxane, 70-110 deg C
Solvent: dioxane or THF or DMF or toluene or DMSO
Literature reference: 10.1021/ol0171463 and 10.1021/jo202472k and 10.1021/jm051065l and 10.1021/acs.oprd.2c00057 (industrial application)



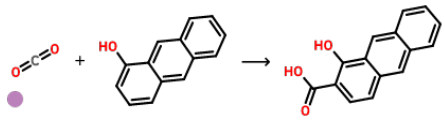
Reaction name: Suzuki Aryl-Aryl Coupling
Reaction conditions: [Pd]-catalyst, ligand, base
Solvent: dioxane
Alternative Solvent: CPME
Literature reference: 10.1126/science.aaa5414 and 10.1021/cr100346g



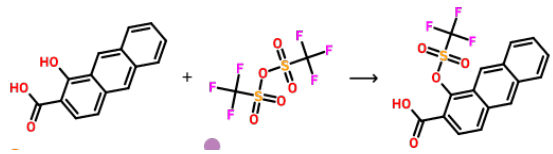
Path #4

Score: 11.50 Estimated cost ($/g): 349.77

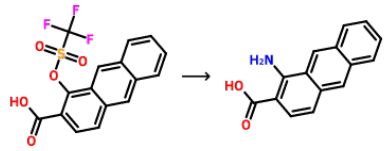
Reaction name: Kolbe–Schmitt reaction
Reaction conditions: CO2, K2CO3
Solvent: water
Literature reference: 10.1016/j.farmac.2003.08.001 and 10.1021/jm980043e and Ullmann's Encyclopedia of Industrial Chemistry, 2005, ch. Phenol, p.3 (10.1002/14356007.a19_299.pub2) and 10.1021/op050045q (industrial application) and US2534022 (industrial application)



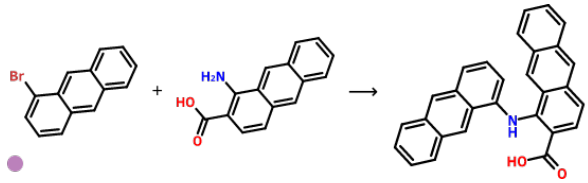
Reaction name: O-sulfonylation
Reaction conditions: NEt3
Solvent: DCM or toluene
Literature reference: 10.1016/j.bmcl.2011.02.024 and 10.1055/s-1998-2113 (experimental)



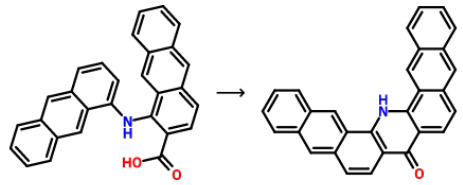
Reaction name: Buchwald Hartwig Amination
Reaction conditions: NH3, Pd[(o-tol)3P]2, NaOtBu, CyPF-t-Bu, dioxane
Solvent: dioxane
Alternative Solvent: CPME
Literature reference: 10.1021/ja903049z and 10.1021/ol401612c and 10.1021/ol501739g and 10.1021/op8000146 and WO2008133459 (Preparation Examples 9-14) and EP2149555 (Synthesis Example 7)



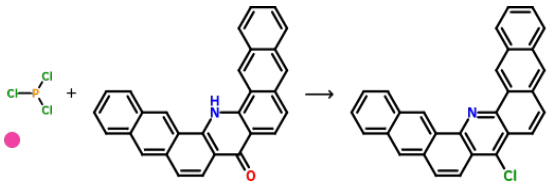
Reaction name: Buchwald-Hartwig Amination with Aromatic Amines
Reaction conditions: [Pd]-catalyst, ligand, Cs2CO3, dioxane or [Pd]-catalyst, ligand, KOtBU, dioxane
Solvent: dioxane or toluene
Literature reference: DOI: 10.1021/jo991699y and 10.1002/anie.200601612 and 10.1038/s41586-018-0056-8 and 10.1021/acs.chemrev.6b00512 and 10.1021/op8000146



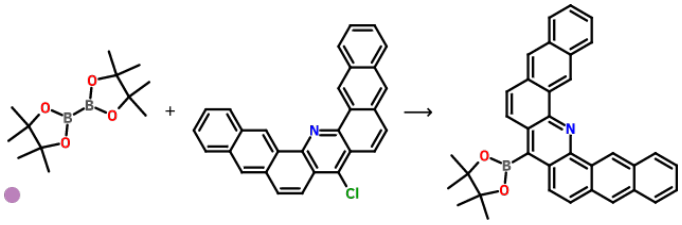
Reaction name: Formation of acridine
Reaction conditions: PPA
Solvent: none
Literature reference: 10.1055/s-1985-31164 (multigram-scale application)



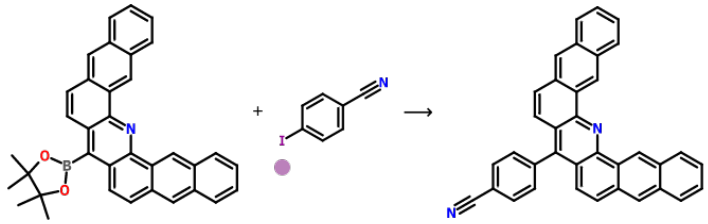
Reaction name: Nucleophilic aromatic chlorination
Reaction conditions: PCl3, DMF
Solvent: DMF
Alternative Solvent: DMSO
Literature reference: 10.1021/jm051146h and 10.1016/j.bmc.2013.06.026 and 10.1016/j.ejmech.2010.05.030



Reaction name: Coupling of B2(pin)2 with aryl halide
Reaction conditions: Pd-cat, AcOK, 1,4-dioxane, 70-110 deg C
Solvent: dioxane or THF or DMF or toluene or DMSO
Literature reference: 10.1021/ol0171463 and 10.1021/jo202472k and 10.1021/jm051065l and 10.1021/acs.oprd.2c00057 (industrial application)



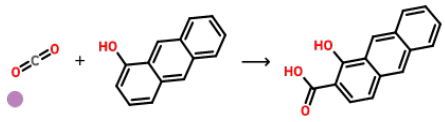
Reaction name: Suzuki Aryl-Aryl Coupling
Reaction conditions: [Pd]-catalyst, ligand, base
Solvent: dioxane
Alternative Solvent: CPME
Literature reference: 10.1126/science.aaa5414 and 10.1021/cr100346g



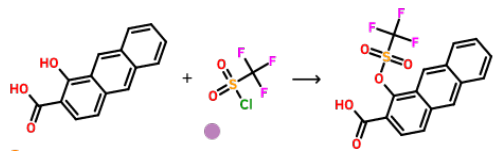
Path #5

Score: 11.50 Estimated cost ($/g): 341.93

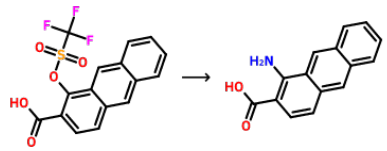
Reaction name: Kolbe–Schmitt reaction
Reaction conditions: CO2, K2CO3
Solvent: water
Literature reference: 10.1016/j.farmac.2003.08.001 and 10.1021/jm980043e and Ullmann's Encyclopedia of Industrial Chemistry, 2005, ch. Phenol, p.3 (10.1002/14356007.a19_299.pub2) and 10.1021/op050045q (industrial application) and US2534022 (industrial application)



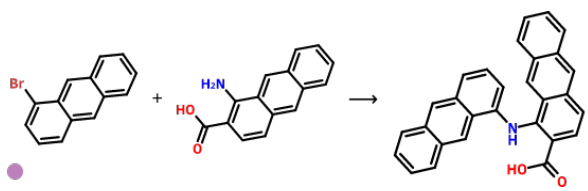
Reaction name: O-sulfonylation
Reaction conditions: NEt3
Solvent: DCM or THF
Alternative Solvent: t-Butyl ethyl ether
Literature reference: 10.1081/SCC-120030306 and 10.1002/ejoc.200900067 (experimental)



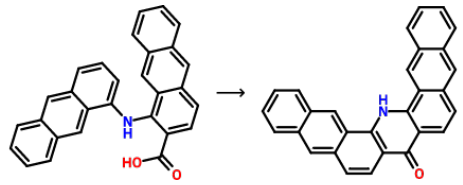
Reaction name: Buchwald Hartwig Amination
Reaction conditions: NH3, Pd[(o-tol)3P]2, NaOtBu, CyPF-t-Bu, dioxane
Solvent: dioxane
Alternative Solvent: CPME
Literature reference: 10.1021/ja903049z and 10.1021/ol401612c and 10.1021/ol501739g and 10.1021/op8000146 and WO2008133459 (Preparation Examples 9-14) and EP2149555 (Synthesis Example 7)



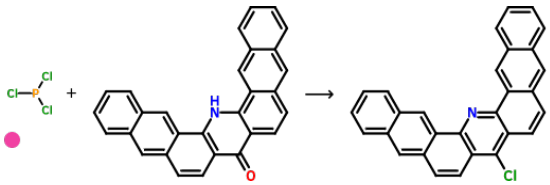
Reaction name: Buchwald-Hartwig Amination with Aromatic Amines
Reaction conditions: [Pd]-catalyst, ligand, Cs2CO3, dioxane or [Pd]-catalyst, ligand, KOtBU, dioxane
Solvent: dioxane or toluene
Literature reference: DOI: 10.1021/jo991699y and 10.1002/anie.200601612 and 10.1038/s41586-018-0056-8 and 10.1021/acs.chemrev.6b00512 and 10.1021/op8000146



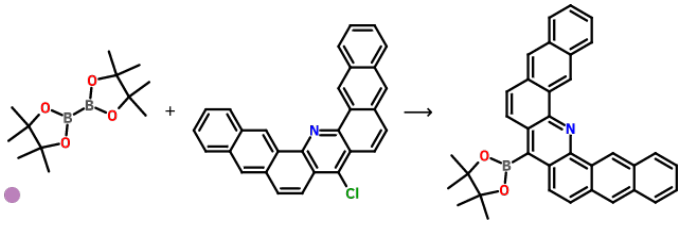
Reaction name: Formation of acridine
Reaction conditions: PPA
Solvent: none
Literature reference: 10.1055/s-1985-31164 (multigram-scale application)



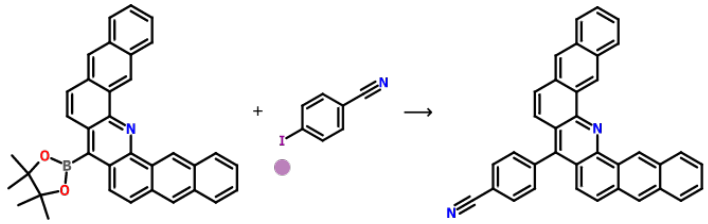
Reaction name: Nucleophilic aromatic chlorination
Reaction conditions: PCl3, DMF
Solvent: DMF
Alternative Solvent: DMSO
Literature reference: 10.1021/jm051146h and 10.1016/j.bmc.2013.06.026 and 10.1016/j.ejmech.2010.05.030



Reaction name: Coupling of B2(pin)2 with aryl halide
Reaction conditions: Pd-cat, AcOK, 1,4-dioxane, 70-110 deg C
Solvent: dioxane or THF or DMF or toluene or DMSO
Literature reference: 10.1021/ol0171463 and 10.1021/jo202472k and 10.1021/jm051065l and 10.1021/acs.oprd.2c00057 (industrial application)



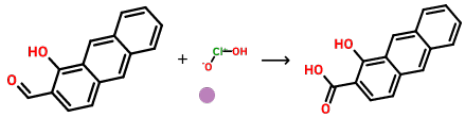
Reaction name: Suzuki Aryl-Aryl Coupling
Reaction conditions: [Pd]-catalyst, ligand, base
Solvent: dioxane
Alternative Solvent: CPME
Literature reference: 10.1126/science.aaa5414 and 10.1021/cr100346g



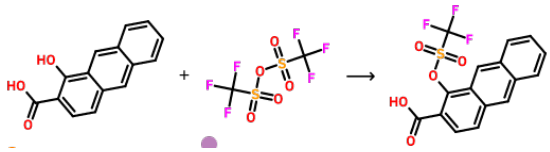
Path #6

Score: 12.00 Estimated cost ($/g): 614.74

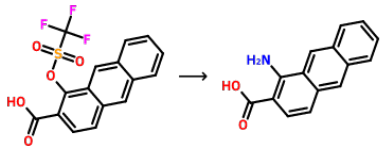
Reaction name: Pinnick oxidation
Reaction conditions: NaClO2, tBuOH, NaH2PO4, 2-methyl-2-butene
Solvent: water
Literature reference: 10.1021/ol401115a and 10.1055/s-2006-942426 and 10.1021/cr040679f (large-scale application)



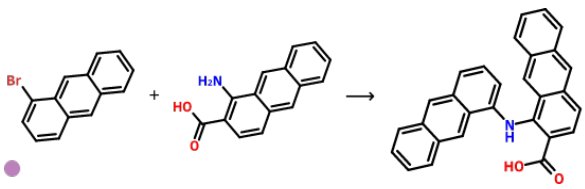
Reaction name: O-sulfonylation
Reaction conditions: NEt3
Solvent: DCM or toluene
Literature reference: 10.1016/j.bmcl.2011.02.024 and 10.1055/s-1998-2113 (experimental)



Reaction name: Buchwald Hartwig Amination
Reaction conditions: NH3, Pd[(o-tol)3P]2, NaOtBu, CyPF-t-Bu, dioxane
Solvent: dioxane
Alternative Solvent: CPME
Literature reference: 10.1021/ja903049z and 10.1021/ol401612c and 10.1021/ol501739g and 10.1021/op8000146 and WO2008133459 (Preparation Examples 9-14) and EP2149555 (Synthesis Example 7)

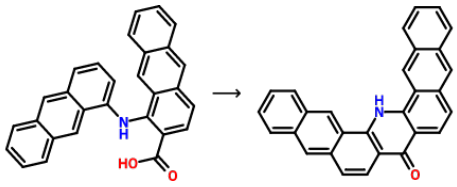


Reaction name: Buchwald-Hartwig Amination with Aromatic Amines
Reaction conditions: [Pd]-catalyst, ligand, Cs2CO3, dioxane or [Pd]-catalyst, ligand, KOtBU, dioxane
Solvent: dioxane or toluene
Literature reference: DOI: 10.1021/jo991699y and 10.1002/anie.200601612 and 10.1038/s41586-018-0056-8 and 10.1021/acs.chemrev.6b00512 and 10.1021/op8000146

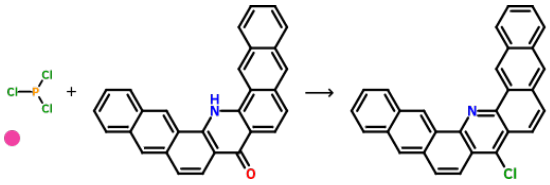


Reaction name: Formation of acridine

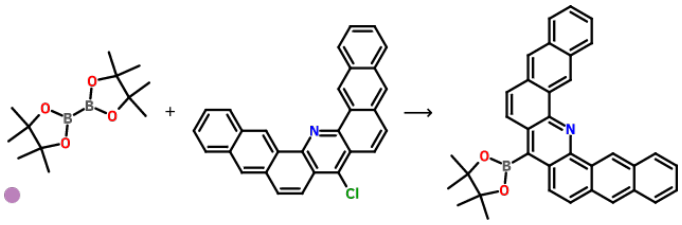
Reaction conditions: PPA
Solvent: none
Literature reference: 10.1055/s-1985-31164 (multigram-scale application)



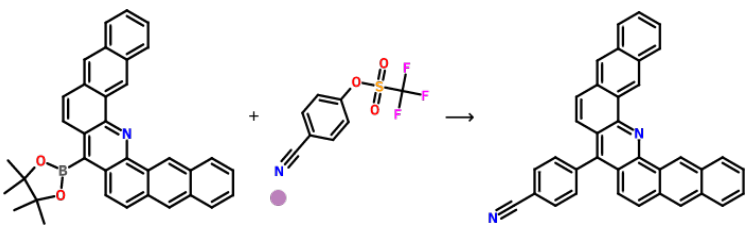
Reaction name: Nucleophilic aromatic chlorination
Reaction conditions: PCl3, DMF
Solvent: DMF
Alternative Solvent: DMSO
Literature reference: 10.1021/jm051146h and 10.1016/j.bmc.2013.06.026 and 10.1016/j.ejmech.2010.05.030



Reaction name: Coupling of B2(pin)2 with aryl halide
Reaction conditions: Pd-cat, AcOK, 1,4-dioxane, 70-110 deg C
Solvent: dioxane or THF or DMF or toluene or DMSO
Literature reference: 10.1021/ol0171463 and 10.1021/jo202472k and 10.1021/jm051065l and 10.1021/acs.oprd.2c00057 (industrial application)



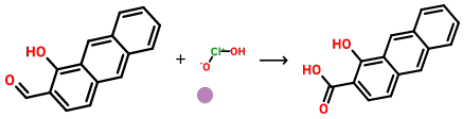
Reaction name: Suzuki Aryl-Aryl Coupling
Reaction conditions: [Pd]-catalyst, ligand, base
Solvent: dioxane
Alternative Solvent: CPME
Literature reference: 10.1126/science.aaa5414 and 10.1021/cr100346g



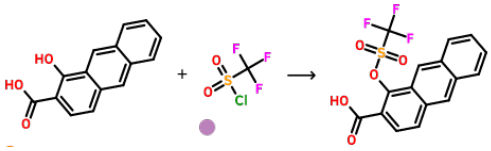
Path #7

Score: 12.00 Estimated cost ($/g): 606.90

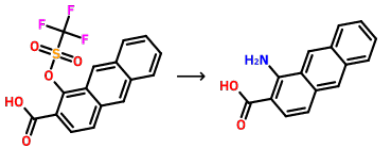
Reaction name: Pinnick oxidation
Reaction conditions: NaClO2, tBuOH, NaH2PO4, 2-methyl-2-butene
Solvent: water
Literature reference: 10.1021/ol401115a and 10.1055/s-2006-942426 and 10.1021/cr040679f (large-scale application)



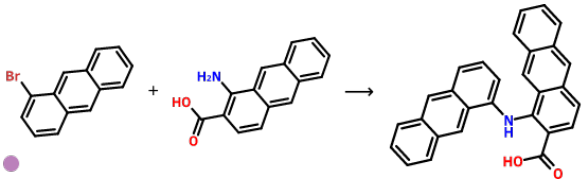
Reaction name: O-sulfonylation
Reaction conditions: NEt3
Solvent: DCM or THF
Alternative Solvent: t-Butyl ethyl ether
Literature reference: 10.1081/SCC-120030306 and 10.1002/ejoc.200900067 (experimental)



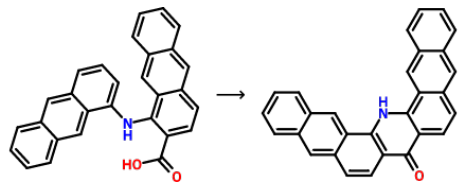
Reaction name: Buchwald Hartwig Amination
Reaction conditions: NH3, Pd[(o-tol)3P]2, NaOtBu, CyPF-t-Bu, dioxane
Solvent: dioxane
Alternative Solvent: CPME
Literature reference: 10.1021/ja903049z and 10.1021/ol401612c and 10.1021/ol501739g and 10.1021/op8000146 and WO2008133459 (Preparation Examples 9-14) and EP2149555 (Synthesis Example 7)



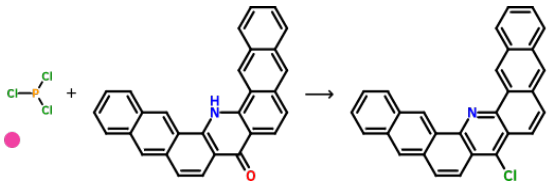
Reaction name: Buchwald-Hartwig Amination with Aromatic Amines
Reaction conditions: [Pd]-catalyst, ligand, Cs2CO3, dioxane or [Pd]-catalyst, ligand, KOtBU, dioxane
Solvent: dioxane or toluene
Literature reference: DOI: 10.1021/jo991699y and 10.1002/anie.200601612 and 10.1038/s41586-018-0056-8 and 10.1021/acs.chemrev.6b00512 and 10.1021/op8000146



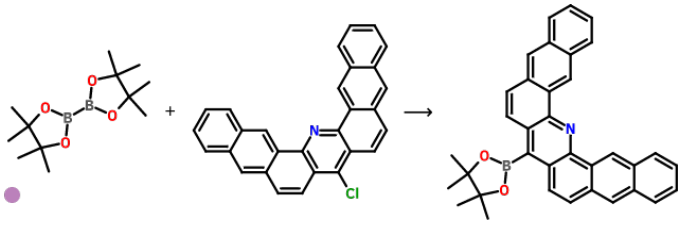
Reaction name: Formation of acridine
Reaction conditions: PPA
Solvent: none
Literature reference: 10.1055/s-1985-31164 (multigram-scale application)



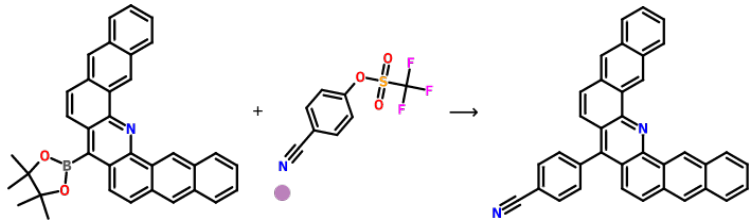
Reaction name: Nucleophilic aromatic chlorination
Reaction conditions: PCl3, DMF
Solvent: DMF
Alternative Solvent: DMSO
Literature reference: 10.1021/jm051146h and 10.1016/j.bmc.2013.06.026 and 10.1016/j.ejmech.2010.05.030



Reaction name: Coupling of B2(pin)2 with aryl halide
Reaction conditions: Pd-cat, AcOK, 1,4-dioxane, 70-110 deg C
Solvent: dioxane or THF or DMF or toluene or DMSO
Literature reference: 10.1021/ol0171463 and 10.1021/jo202472k and 10.1021/jm051065l and 10.1021/acs.oprd.2c00057 (industrial application)



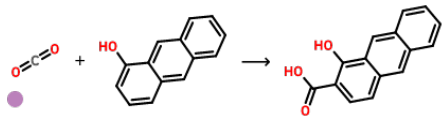
Reaction name: Suzuki Aryl-Aryl Coupling
Reaction conditions: [Pd]-catalyst, ligand, base
Solvent: dioxane
Alternative Solvent: CPME
Literature reference: 10.1126/science.aaa5414 and 10.1021/cr100346g



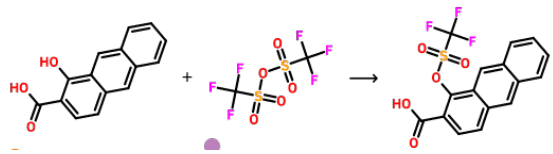
Path #8

Score: 12.00 Estimated cost ($/g): 372.97

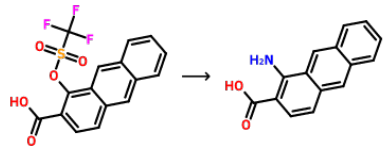
Reaction name: Kolbe–Schmitt reaction
Reaction conditions: CO2, K2CO3
Solvent: water
Literature reference: 10.1016/j.farmac.2003.08.001 and 10.1021/jm980043e and Ullmann's Encyclopedia of Industrial Chemistry, 2005, ch. Phenol, p.3 (10.1002/14356007.a19_299.pub2) and 10.1021/op050045q (industrial application) and US2534022 (industrial application)



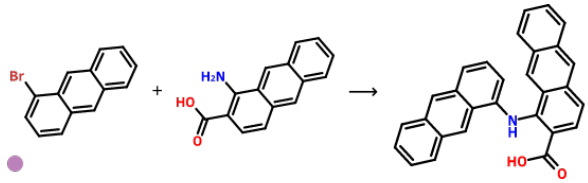
Reaction name: O-sulfonylation
Reaction conditions: NEt3
Solvent: DCM or toluene
Literature reference: 10.1016/j.bmcl.2011.02.024 and 10.1055/s-1998-2113 (experimental)



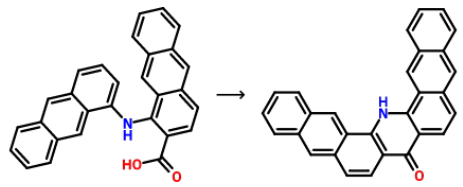
Reaction name: Buchwald Hartwig Amination
Reaction conditions: NH3, Pd[(o-tol)3P]2, NaOtBu, CyPF-t-Bu, dioxane
Solvent: dioxane
Alternative Solvent: CPME
Literature reference: 10.1021/ja903049z and 10.1021/ol401612c and 10.1021/ol501739g and 10.1021/op8000146 and WO2008133459 (Preparation Examples 9-14) and EP2149555 (Synthesis Example 7)



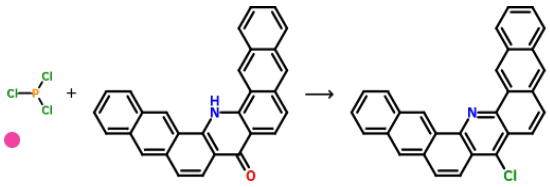
Reaction name: Buchwald-Hartwig Amination with Aromatic Amines
Reaction conditions: [Pd]-catalyst, ligand, Cs2CO3, dioxane or [Pd]-catalyst, ligand, KOtBU, dioxane
Solvent: dioxane or toluene
Literature reference: DOI: 10.1021/jo991699y and 10.1002/anie.200601612 and 10.1038/s41586-018-0056-8 and 10.1021/acs.chemrev.6b00512 and 10.1021/op8000146



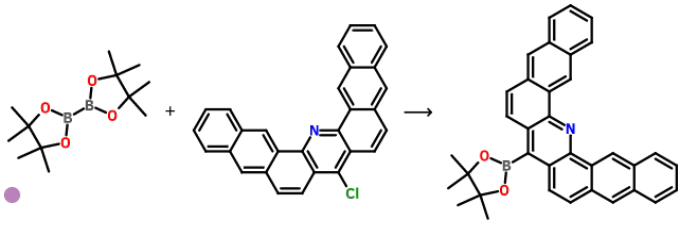
Reaction name: Formation of acridine
Reaction conditions: PPA
Solvent: none
Literature reference: 10.1055/s-1985-31164 (multigram-scale application)



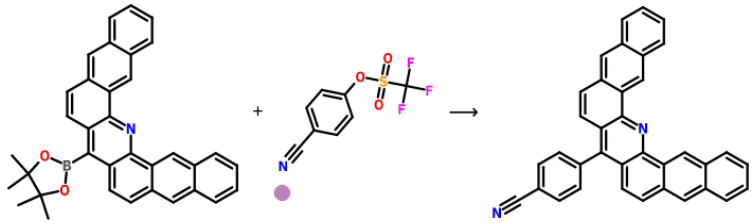
Reaction name: Nucleophilic aromatic chlorination
Reaction conditions: PCl3, DMF
Solvent: DMF
Alternative Solvent: DMSO
Literature reference: 10.1021/jm051146h and 10.1016/j.bmc.2013.06.026 and 10.1016/j.ejmech.2010.05.030



Reaction name: Coupling of B2(pin)2 with aryl halide
Reaction conditions: Pd-cat, AcOK, 1,4-dioxane, 70-110 deg C
Solvent: dioxane or THF or DMF or toluene or DMSO
Literature reference: 10.1021/ol0171463 and 10.1021/jo202472k and 10.1021/jm051065l and 10.1021/acs.oprd.2c00057 (industrial application)



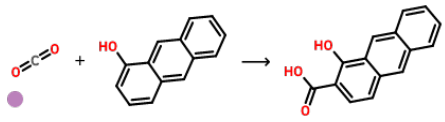
Reaction name: Suzuki Aryl-Aryl Coupling
Reaction conditions: [Pd]-catalyst, ligand, base
Solvent: dioxane
Alternative Solvent: CPME
Literature reference: 10.1126/science.aaa5414 and 10.1021/cr100346g



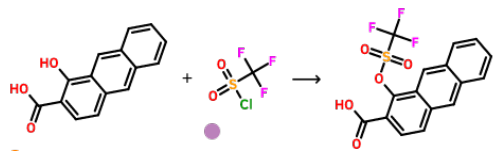
Path #9

Score: 12.00 Estimated cost ($/g): 365.13

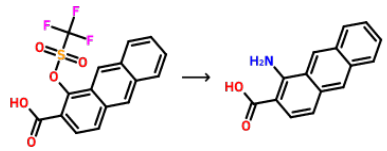
Reaction name: Kolbe–Schmitt reaction
Reaction conditions: CO2, K2CO3
Solvent: water
Literature reference: 10.1016/j.farmac.2003.08.001 and 10.1021/jm980043e and Ullmann's Encyclopedia of Industrial Chemistry, 2005, ch. Phenol, p.3 (10.1002/14356007.a19_299.pub2) and 10.1021/op050045q (industrial application) and US2534022 (industrial application)



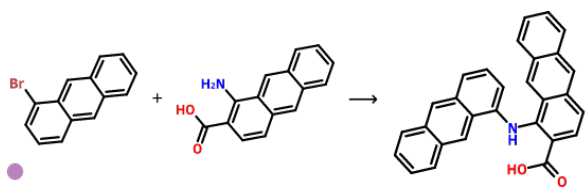
Reaction name: O-sulfonylation
Reaction conditions: NEt3
Solvent: DCM or THF
Alternative Solvent: t-Butyl ethyl ether
Literature reference: 10.1081/SCC-120030306 and 10.1002/ejoc.200900067 (experimental)



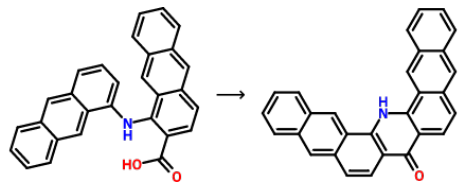
Reaction name: Buchwald Hartwig Amination
Reaction conditions: NH3, Pd[(o-tol)3P]2, NaOtBu, CyPF-t-Bu, dioxane
Solvent: dioxane
Alternative Solvent: CPME
Literature reference: 10.1021/ja903049z and 10.1021/ol401612c and 10.1021/ol501739g and 10.1021/op8000146 and WO2008133459 (Preparation Examples 9-14) and EP2149555 (Synthesis Example 7)



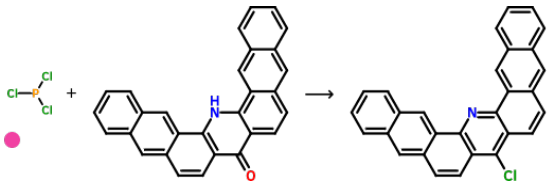
Reaction name: Buchwald-Hartwig Amination with Aromatic Amines
Reaction conditions: [Pd]-catalyst, ligand, Cs2CO3, dioxane or [Pd]-catalyst, ligand, KOtBU, dioxane
Solvent: dioxane or toluene
Literature reference: DOI: 10.1021/jo991699y and 10.1002/anie.200601612 and 10.1038/s41586-018-0056-8 and 10.1021/acs.chemrev.6b00512 and 10.1021/op8000146



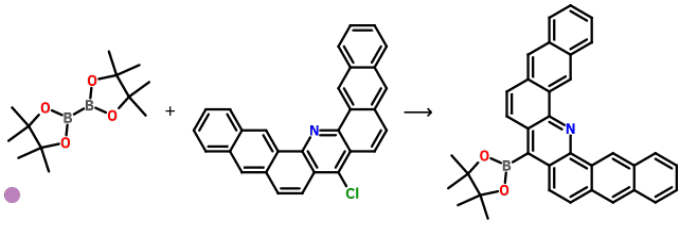
Reaction name: Formation of acridine
Reaction conditions: PPA
Solvent: none
Literature reference: 10.1055/s-1985-31164 (multigram-scale application)



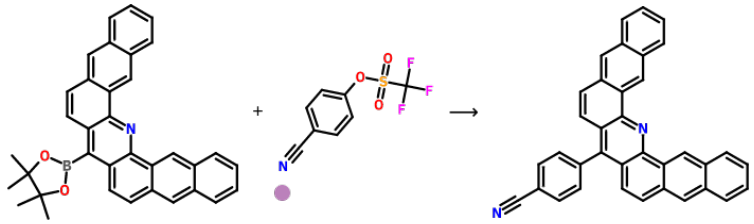
Reaction name: Nucleophilic aromatic chlorination
Reaction conditions: PCl3, DMF
Solvent: DMF
Alternative Solvent: DMSO
Literature reference: 10.1021/jm051146h and 10.1016/j.bmc.2013.06.026 and 10.1016/j.ejmech.2010.05.030



Reaction name: Coupling of B2(pin)2 with aryl halide
Reaction conditions: Pd-cat, AcOK, 1,4-dioxane, 70-110 deg C
Solvent: dioxane or THF or DMF or toluene or DMSO
Literature reference: 10.1021/ol0171463 and 10.1021/jo202472k and 10.1021/jm051065l and 10.1021/acs.oprd.2c00057 (industrial application)



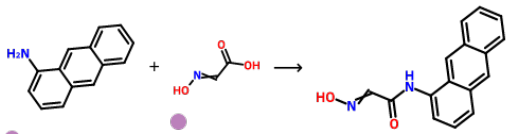
Reaction name: Suzuki Aryl-Aryl Coupling
Reaction conditions: [Pd]-catalyst, ligand, base
Solvent: dioxane
Alternative Solvent: CPME
Literature reference: 10.1126/science.aaa5414 and 10.1021/cr100346g



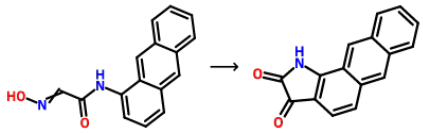
Path #10

Score: 12.00 Estimated cost ($/g): 441.25

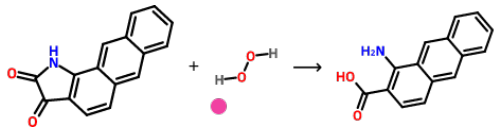
Reaction name: Amide synthesis
Reaction conditions: DCC, DCM, rt or EDCI, DCM, rt
Solvent: DMF or THF
Alternative Solvent: DMSO or t-Butyl ethyl ether
Literature reference: 10.1016/j.bmcl.2013.10.071



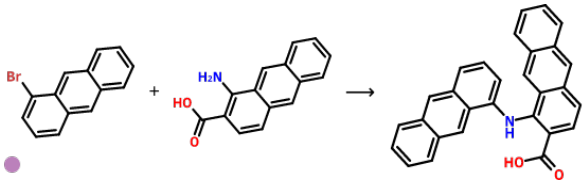
Reaction name: Synthesis of isatin derivatives
Reaction conditions: H2SO4, water, heating
Solvent: water
Literature reference: 10.1021/op100161y and 10.15227/orgsyn.079.0196 and 10.1021/jm060631p and 10.1002/1521-3773(20010518)40:10<1967::AID-ANIE1967>3.0.CO;2-Q and JP2018150285A (all examples)



Reaction name: Oxidative cleavage of isatines
Reaction conditions: NaOH, H2O2, 65 deg C
Solvent: water
Literature reference: 10.1021/op100161y and 10.15227/orgsyn.079.0196 and 10.1016/j.bmc.2015.11.035 and 10.1016/j.tet.2011.05.127

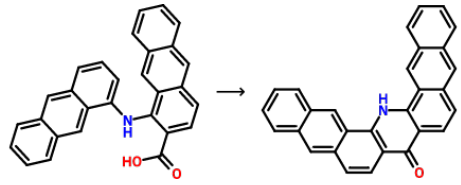


Reaction name: Buchwald-Hartwig Amination with Aromatic Amines
Reaction conditions: [Pd]-catalyst, ligand, Cs2CO3, dioxane or [Pd]-catalyst, ligand, KOtBU, dioxane
Solvent: dioxane or toluene
Literature reference: DOI: 10.1021/jo991699y and 10.1002/anie.200601612 and 10.1038/s41586-018-0056-8 and 10.1021/acs.chemrev.6b00512 and 10.1021/op8000146

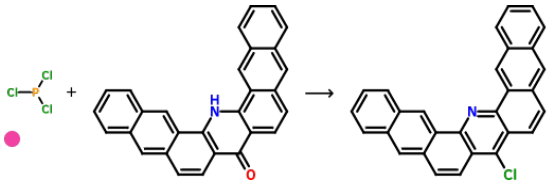


Reaction name: Formation of acridine
Reaction conditions: PPA

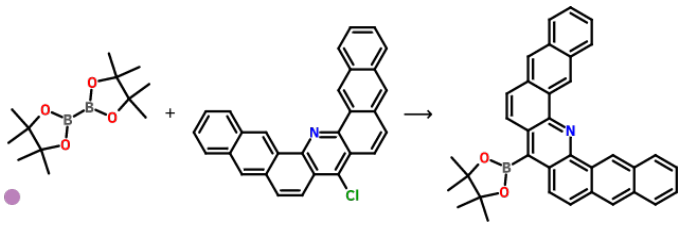
Solvent: none
Literature reference: 10.1055/s-1985-31164 (multigram-scale application)



Reaction name: Nucleophilic aromatic chlorination
Reaction conditions: PCl3, DMF
Solvent: DMF
Alternative Solvent: DMSO
Literature reference: 10.1021/jm051146h and 10.1016/j.bmc.2013.06.026 and 10.1016/j.ejmech.2010.05.030



Reaction name: Coupling of B2(pin)2 with aryl halide
Reaction conditions: Pd-cat, AcOK, 1,4-dioxane, 70-110 deg C
Solvent: dioxane or THF or DMF or toluene or DMSO
Literature reference: 10.1021/ol0171463 and 10.1021/jo202472k and 10.1021/jm051065l and 10.1021/acs.oprd.2c00057 (industrial application)



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