

H-Cube® Quick Start Reaction Guide



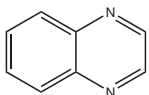
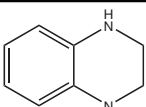
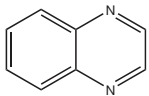
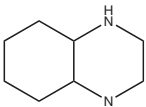

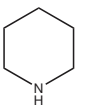
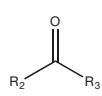
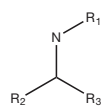
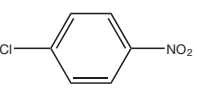
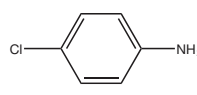
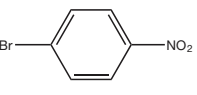
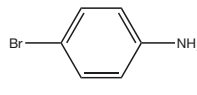
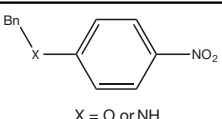
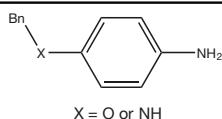
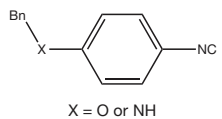
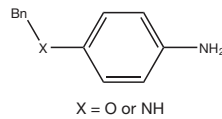
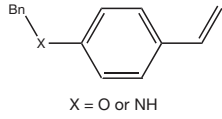
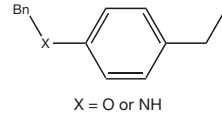
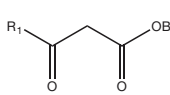
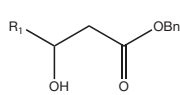
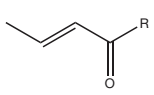
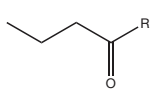
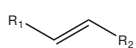
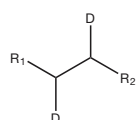
"Good reactions"™



This Quick Start Reaction Guide is designed to give an H-Cube® user the best starting conditions for a particular functional group reduction. The conditions described should give 100% conversion to product in one flow through the system. All reactions should be run at a 0.05 M concentration unless otherwise stated. This sheet will help cut down on your reaction optimization time. Please take into account that every molecule is different and in some cases a small amount of optimization may be necessary.

Reaction Type	Substrate	Product	Recommended Catalyst	Recommended Starting Reaction Conditions
Nitro reduction	<chem>Ar-NO2</chem>	<chem>Ar-NH2</chem>	10% Pd/C and Raney Ni	1.0 mL/min, Full H2 mode, RT to 40°C
Double bond reduction	<chem>H-C(R2)=C(R1)-H</chem>	<chem>R2-CH2-CH2-R1</chem>	10% Pd/C and Raney Ni	1.0 mL/min, Full H2 Mode, RT
	<chem>R3-C(R2)=CH-R1</chem>	<chem>R3-CH2-CH2-R1</chem>	10% Pd/C and Raney Ni	1.0 mL/min, 60 bar, 60°C
Full triple bond reduction	<chem>R2-C#C-R1</chem>	<chem>R2-CH2-CH2-R1</chem>	10% Pd/C and Raney Ni	1.0 mL/min, Full H2 Mode, RT
Z-hydrogenolysis	<chem>R-NH-C(=O)-O-CH2-Ph</chem>	<chem>R-NH2</chem>	20% Pd(OH) ₂ /C or 10% Pd/C	1.0 mL/min, Full H2 mode, 50°C
O-deprotection	<chem>R-O-CH2-Ph</chem>	<chem>R-OH</chem>	20% Pd(OH) ₂ /C or 10% Pd/C	1.0 mL/min, Full H2 mode, 60°C
Amine deprotection	<chem>R-NH-CH2-Ph</chem>	<chem>R-NH2</chem>	20% Pd(OH) ₂ /C or 10% Pd/C	1.0 mL/min, Full H2 mode, 70°C
	<chem>R2-N(R1)-CH2-Ph</chem>	<chem>R2-NH-R1</chem>	20% Pd(OH) ₂ /C or 10% Pd/C and acetic acid	1.0 mL/min, 80 bar, 80°C acetic acid
Nitrile reduction	<chem>R-C#N</chem>	<chem>R-CH2-NH2</chem>	10% Pd/C or Raney Ni	1.0 mL/min, 50 bar, 70°C
Oxime reduction	<chem>R-CH=N-OH</chem>	<chem>R-CH2-NH2</chem>	Raney Ni	1.0 mL/min, 60 bar, 80°C
Aldehyde reduction	<chem>R-CHO</chem>	<chem>R-CH2-OH</chem>	10% Pt/C or Raney Ni	1.0 mL/min, 50 bar, 50°C
Imine reduction	<chem>R2-C(R3)=N-R1</chem>	<chem>R2-CH2-CH2-NH-R1</chem>	10% Pd/C or Raney Ni	1.0 - 2.0 mL/min, Full H2 Mode, 40°C

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Reaction Type	Substrate	Product	Recommended Catalyst	Recommended Starting Reaction Conditions
Selective ring saturation			10% Pd/C	1.0 mL/min, 20 bar, 25°C
Aromatic ring saturation			20% Pd(OH) ₂ /C	1.0 mL/min, 80 bar, 100°C
			5% Rh/C	1.0 mL/min, 80 bar, 100°C acetic acid
Reductive amination	R_1-NH_2 + 		Raney Ni or 10% Pd/C	1.0 mL/min, Full H ₂ Mode, 40°C Use dry solvents. Acetic acid can be used to catalyze reactions with ketones (Never use acetic acid with Raney Ni!)
Selective nitro reduction in the presence of a halogen			5% Ru/C	1.0 mL/min, 70 bar, 75°C
			RuO ₂	2.0 mL/min, 70 bar, 30°C
Selective reduction in the presence of a benzyl protected oxygen or nitrogen			Raney Ni	1.0 mL/min, Full H ₂ Mode, 40°C
			Raney Ni	1.0 mL/min, 50 bar, 70°C
			Raney Ni	1.0 mL/min, Full H ₂ Mode, RT
			10% Pt/C	1.0 mL/min, Full H ₂ Mode, 30°C
Selective double bond reduction in the presence of aldehyde or ketone group			1% Ir/C	1.0 mL/min, Full H ₂ Mode, RT
Reductive dethiation	$R-S-H$	$R-H$	Raney Ni	1.0 mL/min, Full H ₂ Mode, 40°C
Deuteration			10% Pd/C	Use D ₂ O in water reservoir 1.0 mL/min, Full H ₂ Mode, 30°C Only use dry aprotic solvents Do not use H ₂ saturated catalysts

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