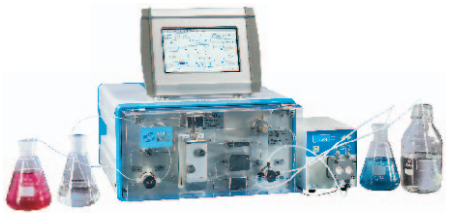
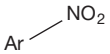
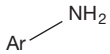
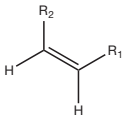
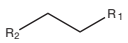
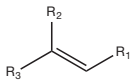
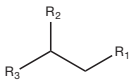
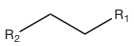
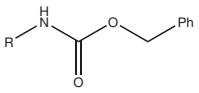
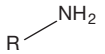
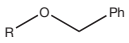
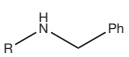
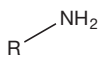
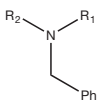
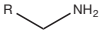
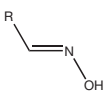
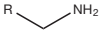
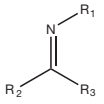
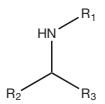
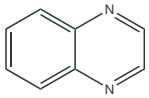
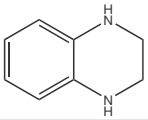
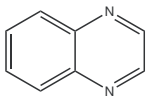
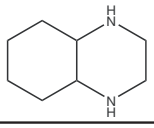
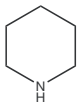
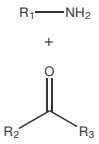
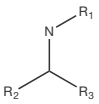
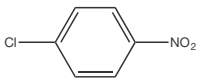
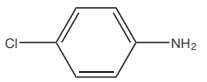
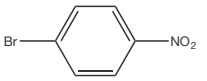
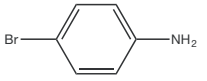
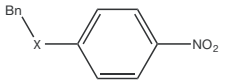
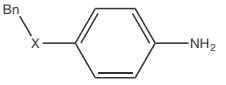
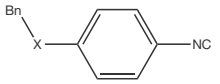
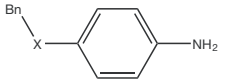
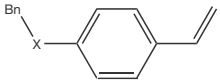
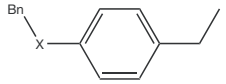
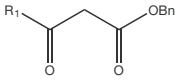
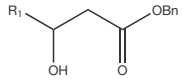
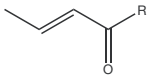
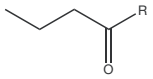
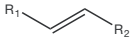
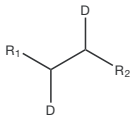
Flow Hydrogenation Quick Start Reaction Guide

This Quick Start Reaction Guide is designed to give an H-Cube Pro™ 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 and 100% H_2 production 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			10% Pd/C or Raney Ni	1.0 mL/min, atm. pressure, RT to 40 °C
Double bond reduction			10% Pd/C or Raney Ni	1.0 mL/min, atm. pressure, RT
			10% Pd/C or Raney Ni	1.0 mL/min, 60 bar, 60 °C
Full triple bond reduction			10% Pd/C or Raney Ni	1.0 mL/min, atm. pressure, RT
Z-hydrogenolysis			20% $Pd(OH)_2/C$ or 10% Pd/C	1.0 mL/min, atm. pressure, 50 °C
O-deprotection			20% $Pd(OH)_2/C$ or 10% Pd/C	1.0 mL/min, atm. pressure, 60 °C
Amine deprotection			20% $Pd(OH)_2/C$ or 10% Pd/C	1.0 mL/min, atm. pressure, 70 °C
			20% $Pd(OH)_2/C$ or 10% Pd/C and acetic acid	1.0 mL/min, 80 bar, 80 °C, acetic acid
Nitrile reduction			10% Pd/C or Raney Ni	1.0 mL/min, 50 bar, 70 °C
Oxime reduction			Raney Ni	1.0 mL/min, 60 bar, 80 °C
Aldehyde reduction			10% Pt/C or Raney Ni	1.0 mL/min, 50 bar, 50°C
Imine reduction			10% Pd/C or Raney Ni	1.0 - 2.0 mL/min, atm. pressure, 40°C

Reaction Type	Substrate	Product	Recommended Catalyst	Recommended Starting Reaction Conditions
Selective ring saturation			10% Pd/C	1.0 mL/min, 20 bar, 25 °C, 7% H_2 production
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			Raney Ni or 10% Pd/C	1.0 mL/min, atm. pressure, 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, 7% H_2 production
			RuO_2	2.0 mL/min, 70 bar, 30 °C, 7% H_2 production
Selective reduction in the presence of a benzyl protected oxygen or nitrogen	 X = O or NH	 X = O or NH	Raney Ni	1.0 mL/min, atm. pressure, 40 °C
	 X = O or NH	 X = O or NH	Raney Ni	1.0 mL/min, 50 bar, 70 °C
	 X = O or NH	 X = O or NH	Raney Ni	1.0 mL/min, atm. pressure, RT
			10% Pt/C	1.0 mL/min, atm. pressure, 30 °C
Selective double bond reduction in the presence of aldehyde or ketone group			1% Ir/C	1.0 mL/min, atm. pressure, RT, 7% H_2 production
Reductive dethionation			Raney Ni	1.0 mL/min, atm. pressure, 40 °C
Deuteration			10% Pd/C	Use D_2O in water reservoir 1.0 mL/min, atm. presure, 30 °C Only use dry aprotic solvents Do not use H_2 saturated catalysts