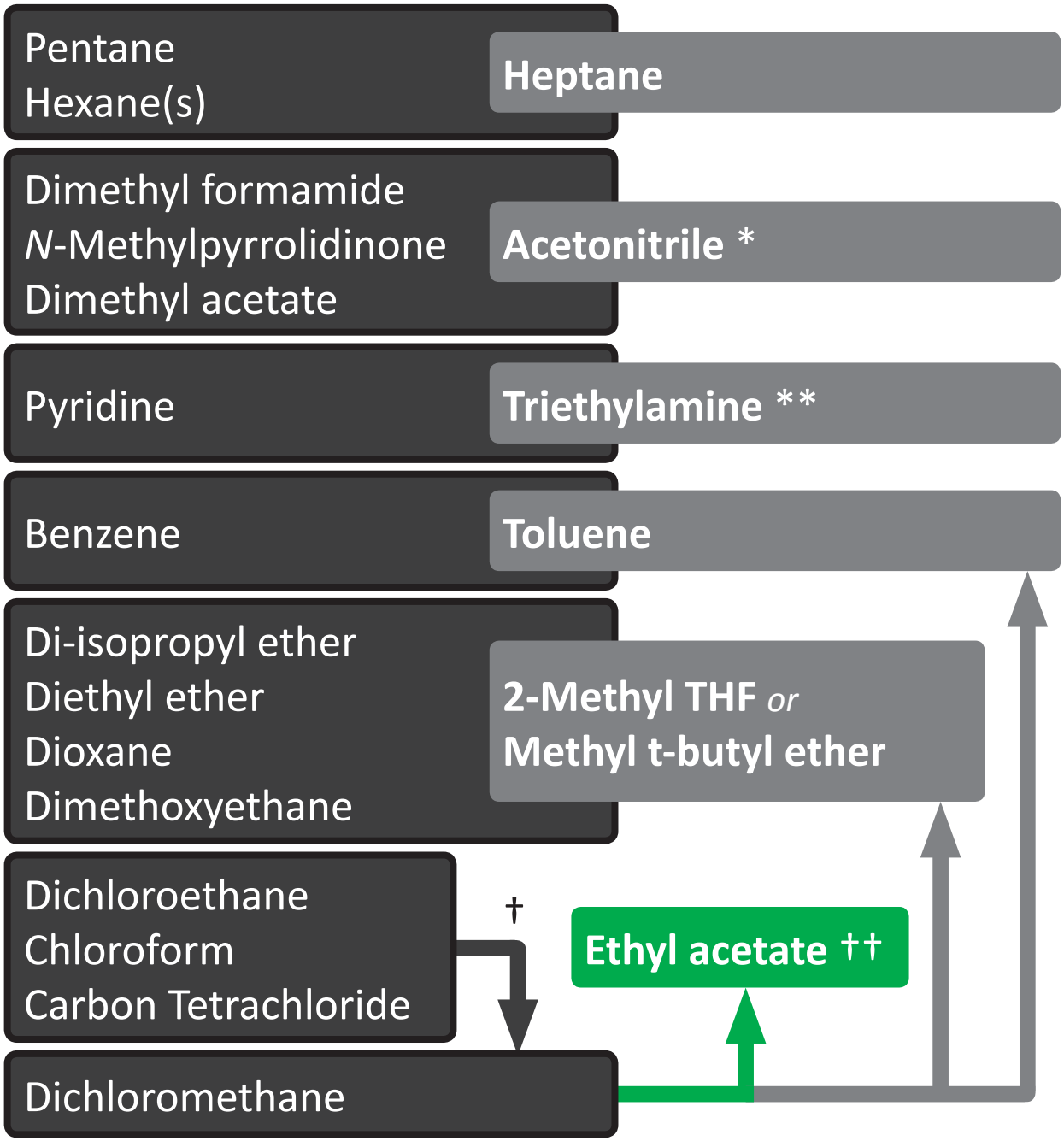
The Good, the Bad and the Ugly

A guide to solvent selection

Preferred	Usable	Undesirable
Water	Cylcohexane	Pentane
Acetone	Heptane	Hexane(s)
Ethanol	Toluene	Di-isopropyl ether
2-Propanol	Methylcyclohexane	Diethyl ether
1-Propanol	Methyl *t*-butyl ether	Dichloromethane
Ethyl acetate	Isooctane	Dichloroethane
Isopropyl acetate	Acetonitrile	Chloroform
Methanol	2-MethylTHF	Dimethyl formamide
Methyl ethyl ketone	Tetrahydrofuran	*N*-Methylpyrrolidinone
1-Butanol	Xylenes	Pyridine
t-Butanol	Dimethyl sulfoxide	Dimethyl acetate
	Acetic acid	Dioxane
	Ethylene glycol	Dimethoxyethane
		Benzene
		Carbon Tetrachloride

Solvent alternatives



* Acetonitrile is a relatively poor substitute for these dipolar aprotic solvents, especially for reactions involving a strong base. Identifying alternatives for this group is an important priority for green chemistry.

** If pyridine is used as a base.

† If a chlorinated solvent needs to be used, dichloromethane is the better choice.

†† If doing chromatography, an Ethyl acetate/heptane mixture is a good substitute for chlorinated solvents.

Principles of Green Chemistry:

Synthetic methods should be designed to use substances that possess little or no toxicity to human health and the environment.

The use of solvents should be made unnecessary whenever possible and, when used, innocuous.

Substances used in a chemical process should be chosen so as to minimise the potential for chemical accidents.

Source:

A study by Pfizer Global Research and Development:
K Alfonsi, J Colberg, P J Dunn, T Fevig, S Jennings,
T A Johnson, H P Kleine, C Knight, M A Nagy, D A Perry and
M Stefaniak. "Green chemistry tools to influence a medicinal chemistry and research chemistry based organisation" *Green Chem.*, 2008, **10**, 31-36.

Poster compiled by Michael Clarke, Centre for Green Chemistry, Monash University. Available online at:

www.greenchem.org