An Investigation into the One-Pot Heck Olefination-Hydrogenation Reaction

Kimberly Geoghegan, Susan Kelleher and Paul Evans*

Centre for Synthesis and Chemical Biology, School of Chemistry and Chemical Biology,

University College Dublin, Dublin 4, Ireland. E-mail: paul.evans@ucd.ie

Contents:	Pg.
Scanned Spectra	S2-32

Proton and carbon NMR spectra:

1-Methyl-8-thia-9-aza-tricyclo[7.2.1.0^{2,7}]dodeca-2(7),3,5-triene 8,8-dioxide **11c** (400 MHz, CDCl₃)

1-Methyl-8-thia-9-aza-tricyclo[7.2.1.0^{2,7}]dodeca-2(7),3,5-triene 8,8-dioxide **11c** (100 MHz, CDCl₃)

1-(2-Bromo-4,5-dimethoxybenzenesulfonyl)-3-methyl-2,5-dihydro-1H-pyrrole **9d** (400 MHz, CDCl₃)

1-(2-Bromo-4,5-dimethoxybenzenesulfonyl)-3-methyl-2,5-dihydro-1*H*-pyrrole **9d** (100 MHz, CDCl₃)

4,5-Dimethoxy-1-methyl-8-thia-9-aza-tricyclo[7.2.1.0^{2,7}]dodeca-2(7),3,5,10-tetraene 8,8-dioxide **10d** (400 MHz, CDCl₃)

4,5-Dimethoxy-1-methyl-8-thia-9-aza-tricyclo[7.2.1.0^{2,7}]dodeca-2(7),3,5,10-tetraene 8,8-dioxide **10d** (100 MHz, CDCl₃)

4,5-Dimethoxy-1-methyl-8-thia-9-aza-tricyclo[7.2.1.0^{2,7}]dodeca-2(7),3,5-triene 8,8-dioxide **11d** (400 MHz, CDCl₃)

4,5-Dimethoxy-1-methyl-8-thia-9-aza-tricyclo[7.2.1.0^{2,7}]dodeca-2(7),3,5-triene 8,8-dioxide **11d** (100 MHz, CDCl₃)

1-(2-Bromobenzenesulfonyl)-2,4,5,6,7,7a-hexahydro-1*H*-indole **9e** (400 MHz, CDCl₃)

1-(2-Bromobenzenesulfonyl)-2,4,5,6,7,7a-hexahydro-1*H*-indole **9e** (100 MHz, CDCl₃)

(±)-(4a*R*,10a*S*)-4a,10-etheno-2,3,4a,10,10a-hexahydro-1*H*-9-thia-10-azaphenanthrene 9,9-dioxide **10e** (400 MHz, CDCl₃)

(±)-(4a*R*,10a*S*)-4a,10-etheno-2,3,4,4a,10,10a-hexahydro-1*H*-9-thia-10-azaphenanthrene 9,9-dioxide **10e** (100 MHz, CDCl₃)

(±)-(4a*R*,10a*S*)-4a,10-ethano-2,3,4a,10,10a-hexahydro-1*H*-9-thia-10-azaphenanthrene 9,9-dioxide **11e** (400 MHz, CDCl₃)

(±)-(4a*R*,10a*S*)-4a,10-ethano-2,3,4a,10,10a-hexahydro-1*H*-9-thia-10-azaphenanthrene 9,9-dioxide **11e** (100 MHz, CDCl₃)

2-Phenyltetrahydrofuran **15h** (400 MHz, CDCl₃)

2-Phenyltetrahydrofuran **15h** (100 MHz, CDCl₃)

Methyl 3-(1-naphthyl)propanoate **17a** (400 MHz, CDCl₃)

Methyl 3-(1-naphthyl)propanoate **17a** (100 MHz, CDCl₃)

Methyl 5-(3,4-dimethoxyphenyl)pentanoate **17f** (400 MHz, CDCl₃)

Methyl 5-(3,4-dimethoxyphenyl)pentanoate **17f** (125 MHz, CDCl₃)

Methyl 3-(pyridin-3-yl)propanoate **17i** (500 MHz, CDCl₃)

Methyl 3-(pyridin-3-yl)propanoate **17i** (125 MHz, CDCl₃)

Methyl 3-(1,2,3,4-tetrahydroquinolin-3-yl)propanoate **17j** (400 MHz, CDCl₃)

Methyl 3-(1,2,3,4-tetrahydroquinolin-3-yl)propanoate **17j** (100 MHz, CDCl₃)

Methyl 3-(3-(trifluoromethyl)phenyl)propanoate **17k** (400 MHz, CDCl₃)

Methyl 3-(3-(trifluoromethyl)phenyl)propanoate **17k** (100 MHz, CDCl₃)

(*R*)-*N*-(1-(Naphthalen-1-yl)ethyl)-3-(3-(trifluoromethyl)phenyl)propanamide **18** (400 MHz, CDCl₃)

(*R*)-*N*-(1-(Naphthalen-1-yl)ethyl)-3-(3-(trifluoromethyl)phenyl)propanamide **18** (100 MHz, CDCl₃)

(*R*)-*N*-(1-(Naphthalen-1-yl)ethyl)-3-(3-(trifluoromethyl)phenyl)propan-1-amine (Sensipar) **19** (400 MHz, CDCl₃)

(*R*)-*N*-(1-(Naphthalen-1-yl)ethyl)-3-(3-(trifluoromethyl)phenyl)propan-1-amine (Sensipar) **19** (100 MHz, CDCl₃)

Mixture of methyl 3,3-diphenylacrylate **20** and 3-Phenylpropionic acid methyl ester **15a** (400 MHz, CDCl₃)