

# Report of the President 2009/2010

Sep 2009 - Aug 2010

Research Publications for the School of Chemistry & Chemical Biology

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## Book Chapters

### [Dr Francesca Paradisi](#)

Engel, P.C and Paradisi, F. (2010) 'Novel enzymes for biotransformation and resolution of alpha-amino acids' In: J.C Vederas (eds). *Comprehensive Natural Product 2 Chemistry and Biology*. Oxford: Elsevier.

Conway,P. and Paradisi, F. and Engel, P.C. (2010) 'Synthesis of substituted derivatives of L-phenylalanine and of other non-natural L-amino acids using engineered mutants of phenylalanine dehydrogenase' In: John Whittall & Peter W. Sutton (eds). *Practical Methods in Biocatalysis and Biotransformations*. Oxford: John Wiley.

## Peer Reviewed Journals

### [Professor Martin Albrecht](#)

J. A. Kitchen, C. Gandolfi, M. Albrecht, G. N. Jameson, J. L. Talloon, S. Brooker (2010) 'The Tail that Wags the Dog: Room-Temperature Spin Crossover and Langmuir-Blodgett Film Formation of an Iron(II) Triazole Complex Featuring a Long Alkyl Chain Substituent'. *Chemical Communications*, 46 :6464-6466.

L. Mercs, M. Albrecht (2010) 'Beyond Catalysis: N-Heterocyclic Carbene Complexes as Components for Medicinal, Luminescent, and Functional Materials Applications'. *Chemical Society Reviews*, 39 :1903-1912.

C. Gandolfi, N. Miyashita, D. G. Kurth, P. N. Martinho, G. G. Morgan, M. Albrecht (2010) 'Organization of Spin- and Redox-Labile Metal Centers into Langmuir and Langmuir-blodgett Films'. *Dalton Transactions*, 39 :4508-4516.

Schuster, O, Mercs, L, Albrecht, M (2010) 'The Potential of N-Heterocyclic Carbene Complexes as Components for Electronically Active Materials'. *Chimia*, 64 :184-187

P. N. Martinho, C. J. Harding, H. Müller-Bunz, M. Albrecht, G. G. Morgan (2010) 'Tuning Spin Crossover in Amphiphilic Iron(III) Complexes'. *European Journal of Inorganic Chemistry*, :675-679.

N. G. White, H. L. C. Feltham, C. Gandolfi, M. Albrecht, S. Brooker (2010) 'Towards Langmuir-Blodgett Films of Magnetically Interesting Materials: Solution High Spin/Low Spin Equilibrium in Amphiphilic Iron(II) Complexes of a Triazole-Containing Ligand'. *Dalton Transactions*, 39 :3751-3758.

Schuster, O, Mercs, L, Albrecht, M (2010) 'The Potential of N-Heterocyclic Carbene Complexes as Components for Electronically Active Materials'. *Chimia*, 64 :184-187.

M. Albrecht (2010) 'Cyclometalation Using d-Block Transition Metals: Fundamental Aspects and Recent Trends'. *Chemical Reviews*, 110 :576-623.

Iglesias, M,Albrecht, M (2010) 'Expanding the family of mesoionic complexes: donor properties and catalytic impact of palladated isoxazolyldenes'. *Dalton Transactions*, 39 :5213-5215.

A. Krüger, A. Neels, M. Albrecht (2010) 'Rhodium-Mediated Activation of an Alkane-type C-H Bond'. *Chemical Communications*, 46 :315-317.

M. Albrecht (2009) 'Carbenes in Action'. *Science*, 326 :532-533.

#### Dr Vitaly Buckin

Ochendusko, A,Buckin, V (2010) 'Real-Time Monitoring of Heat-Induced Aggregation of beta-Lactoglobulin in Aqueous Solutions Using High-Resolution Ultrasonic Spectroscopy'. *International Journal Of Thermophysics*, 31 :113-130.

Hickey, S,Hagan, SA,Kudryashov, E,Buckin, V (2010) 'Analysis of phase diagram and microstructural transitions in an ethyl oleate/water/Tween 80/Span 20 microemulsion system using high-resolution ultrasonic spectroscopy'. *International Journal of Pharmaceutics*, 388 :213-222.

#### Professor Kenneth A Dawson

Cabaleiro-Lago, C,Quinlan-Pluck, F,Lynch, I,Dawson, KA,Linse, S (2010) 'Dual Effect of Amino Modified Polystyrene Nanoparticles on Amyloid beta Protein Fibrillation'. *Neuroscience*, 1 :279-287.

Miller, IS,Lynch, I,Dowling, D,Dawson, KA,Gallagher, WM (2010) 'Surface-induced cell signaling events control actin rearrangements and motility'. *Journal of Biomedical Materials Research Part A*, 93A :493-504.

Montes-Burgos, I,Walczyk, D,Hole, P,Smith, J,Lynch, I,Dawson, K (2010) 'Characterisation of nanoparticle size and state prior to nanotoxicological studies'. *Journal Of Nanoparticle Research*, 12 :47-53.

Walczyk, D,Bombelli, FB,Monopoli, MP,Lynch, I,Dawson, KA (2010) 'What the Cell Sees in Bionanoscience'. *Journal of the American Chemical Society*, 132 :5761-5768.

Cabaleiro-Lago, C,Lynch, I,Dawson, KA,Linse, S (2010) 'Inhibition of IAPP and IAPP((20-29)) Fibrillation by Polymeric Nanoparticles'. *Langmuir*, 26 :3453-3461.

de Jong WH, Park MV, Annema W, Salvati A, Lesniak A, Elsaesser A, Barnes C, McKerr G, Howard CV, Lynch I, Dawson KA, Piersma AH, (2009) 'In vitro developmental toxicity test detects inhibition of stem cell differentiation by silica nanoparticles'. *Toxicology and Applied Pharmacology*, 240 (1):108-116.

Dawson KA, Lynch I, Salvati A, (2009) 'Protein-nanoparticle interactions: What does the cell see?'. *Nature nanotechnology*, 4 (9):546-547.

### Dr Paul Evans

Morgan BS, O'Byrne A, Murray C, Keegan D, Palacio C, Evans P, (2010) 'The thio-adduct facilitated, enzymatic kinetic resolution of 4-hydroxycyclopentenone and 4-hydroxycyclohexenone'. *Organic and Biomolecular Chemistry*, 8 (3):539-545.

Evans P, Klein JE, Geoghegan K, MÃ©ral N, (2010) 'Selective generation of quaternary all-carbon-centres through Heck-cyclisations: synthesis of mesembrane'. *Chemical Communications*, 46 (6):937-939.

Evans P, McLaughlin NP, (2010) 'Dihydroxylation of vinyl sulfones: stereoselective synthesis of (+)- and (-)-febrifugine and halofuginone'. *Journal of Organic Chemistry*, 75 (2):518-521.

Evans P, Kelleher S, Quesne PY, (2009) 'Diastereoselective functionalisation of benzo-annulated bicyclic sultams: Application for the synthesis of cis-2,4-diarylpyrrolidines'. *Journal of Organic Chemistry*, 5 .

J. E. M. N. Klein, H. Müller-Bunz and P. Evans, *Studies Concerning the Electrophile Amino-Alkene Cyclisation for the Synthesis of Bicyclic Amines*, *Org. Biomol. Chem.*, **2009**, 7, 986.

Y. Kavanagh, M. O'Brien and P. Evans, *Stereocontrolled Preparation of Bicyclic Alkaloid Analogues: An Approach Towards the Kinabalurine Skeleton*, *Tetrahedron*, **2009**, 65, 8259.

S. A. Brusey, E. V. Banide, S. Dörrich, P. O'Donohue, Y. Ortin, H. Müller-Bunz, C. Long, P. Evans and M. J. McGlinchey, *An X-Ray Crystallographic and NMR Spectroscopic Study of ( $\eta^2$ -Alkene( $\mu$ -alkyne)pentacarbonyldicobalt Complexes: Arrested Pauson-Khand Reaction Intermediates*, *Organometallics*, **2009**, 28, 6308.

E. Dunny and P. Evans, *Stereocontrolled Synthesis of the PPAR- $\gamma$  Agonist 10-Nitrolinoleic Acid*, *J. Org. Chem.*, **2010**, 75, 5334.

N. P. McLaughlin, E. Butler, P. Evans, N. P. Brunton, A. Koidis and D. Rai, *A Short Synthesis of (+)- and (-)-Falcarinol*, *Tetrahedron*, **2010**, 66, 9681.

### Dr Hasim Ibrahim

Akula, R, Galligan, M, Ibrahim, H (2009) 'Umpolung of halide reactivity: efficient (diacetoxyiodo)benzene-mediated electrophilic alpha-halogenation of 1,3-dicarbonyl compounds'. *Chemical Communications*, :6991-6993.

### Professor Michael James McGlinchey

Nikitin, K, Ortin, Y, Muller-Bunz, H, Plamont, MA, Jaouen, G, Vessieres, A, McGlinchey, MJ (2010) 'Organometallic SERMs (selective estrogen receptor modulators): Cobaltifens, the (cyclobutadiene)cobalt analogues of hydroxytamoxifen'.

*J ORGANOMET CHEM*, 695 :595-608.

Oulie, P, Altes, L, Milosevic, S, Bouteille, R, Muller-Bunz, H, McGlinchey, MJ (2010) 'Different Reactivity Patterns of Trimethylsilyl- and Phenyl-Substituted Propargylallenes: Fe-2(CO)(9)- and [Ag](+)-Promoted Cyclizations'. *Meta*, 29 :676-686.

S. Brusey, E. V. Banide, S. Dörrich, P. O'Donohue, C. Long, Y. Ortin, H. Müller-Bunz, P. Evans and M. J. McGlinchey (2009) 'An X-Ray Crystallographic and NMR Spectroscopic Study of ( $\eta^2$  alkene)( $\mu$ -alkyne)pentacarbonyldicobalt complexes: Arrested Pauson-Khand Reaction Intermediates'. *Organometallics*, 28 :6308-6319.

Y. L. K. Tan, P. Pigeon, E. A. Hillard, S. Top, A. Vessières, M. J. McGlinchey, H. Müller-Bunz and Gérard Jaouen (2009) 'Synthesis, oxidation chemistry and cytotoxicity studies on ferrocene derivatives of diethylstilbestro'. *Dalton Transactions*, :10871-10881.

#### [Dr Grace Morgan](#)

Gandolfi, C, Miyashita, N, Kurth, DG, Martinho, PN, Morgan, GG, Albrecht, M (2010) 'Organization of spin- and redox-labile metal centers into Langmuir and Langmuir-Blodgett films'. *Journal of the Chemical Society-Dalton Transactions*, 39 :4508-4516.

Martinho, PN, Harding, CJ, Muller-Bunz, H, Albrecht, M, Morgan, GG (2010) 'Inducing Spin Crossover in Amphiphilic Iron(III) Complexes'. *European Journal of Inorganic Chemistry*, 2010 (5):675-679. →🌐

K. Pandurangan, S. Gallagher, G. G. Morgan, H. Müller-Bunz and F. Paradisi (2010) 'Structure and Antibacterial Activity of the Silver(I) Complex of 2-Aminophenoxazine-3-one'. *Metallomics*, 2 :530-534.

#### [Professor Robert O'Neill](#)

Rothwell, S.A.; Killoran, S.J.; O'Neill, R.D. (2010) 'Enzyme immobilization strategies and electropolymerization conditions to control sensitivity and selectivity parameters of a polymer-enzyme composite glucose biosensor'. *Sensors*, 10 (7):6439-6462. →🌐

Zain, ZM, O'Neill, RD, Lowry, JP, Pierce, KW, Tricklebank, M, Dewa, A, Ab Ghani, S (2010) 'Development of an implantable D-serine biosensor for in vivo monitoring using mammalian D-amino acid oxidase on a poly(o-phenylenediamine) and Nafion-modified platinum-iridium disk electrode'. *Biosensors & Bioelectronics*, 25 :1454-1459.

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#### [Professor Donal O'Shea](#)

Tasior, M, Murtagh, J, Frimannsson, DO, McDonnell, SO, O'Shea, DF (2010) 'Water-solubilised BF<sub>2</sub>-chelated tetraarylazadipyromethenes'. *Org Biomol Chem*, 8 :522-525.

Murtagh, J, Frimannsson, DO, O'Shea, DF (2009) 'Azide Conjugatable and pH Responsive Near-Infrared Fluorescent Imaging Probes'. *Organic Letters*, 11 :5386-5389.

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### **Professor Stefan Oscarson**

Sundgren A, Lahmann M, Oscarson S (2010) 'Synthesis of 6-PEtN-alpha-D-GalpNAc-(1->6)-beta-D-Galp-(1->4)-beta-D-GlcpNAc-(1->3)-beta-D-Galp-(1->4)-beta-D-Glcp, a Haemophilus influenzae lipopolysaccharide structure, and biotin and protein conjugates thereof'. *Beilstein J. Org. Chem.*, 6 No. 80 doi:10.3762/bjoc.6.80.

Fourniere, Viviane, Skantz, Linnea, Sajtos, Ferenc, Oscarson, Stefan, Lahmann, Martina (2010) 'Synthesis of the Lewis b pentasaccharide and a HSA-conjugate thereof'. *Tetrahedron FIELD Full Journal Title:Tetrahedron*, 66 (3939):7850-78557850.

Adrian Meredith, Jenny, Wallberg, Hans, Vrang, Lotta, scarson, Stefan, Parkes, Kevin, Hallberg, Anders, Samuelsson, Bertil (2010) 'Design and synthesis of novel P2 substituents in diol-based HIV protease inhibitors'. *Eur. J. Med. Chem. FIELD Full Journal Title:European Journal of Medicinal Chemistry*, 45 (11):160-170160.

Andre, Sabine, Lahmann, Martina, Gabius, Hans-Joachim, Oscarson, Stefan (2010) 'Glycocluster Design for Improved Avidity and Selectivity in Blocking Human Lectin/Plant Toxin Binding to Glycoproteins and Cells'. *Mol. Pharmaceutics FIELD Full Journal Title:Molecular Pharmaceutics* .

Olsson JD, Oscarson S (2010) 'Synthesis of phosphorylated 3,4-branched trisaccharides corresponding to LPS inner core structures of Neisseria meningitidis and Haemophilus influenzae'. *Carbohydrate research*, 345 (10):1331-1338.

Nurisso A, Blanchard B, Audfray A, Rydner L, Oscarson S, Varrot A, Imberty A (2010) 'Role of water molecules in structure and energetics of Pseudomonas

aeruginosa lectin I interacting with disaccharides'. *Journal of Biological Chemistry*, 285 (26):20316-20327.

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Andersson, CH, Lahmann, M, Oscarson, S, Grennberg, H (2009) 'Reversible non-covalent derivatisation of carbon nanotubes with glycosides'. *Soft Matter*, 5 :2713-2716.

#### [Dr Francesca Paradisi](#)

Moran, S. et al. (2010) 'Production of lipopeptides in *Bacillus* sp. CS93 isolated from Pozol'. *FEMS Microbiol Letters*, 304 :69-73.

Patil, S et al. (2010) 'Synthesis, Cytotoxicity and Antibacterial Studies of p-Methoxybenzyl-Substituted and Benzyl-Substituted N-Heterocyclic Carbene-Silver Complexes'. *European Journal of Inorganic Chemistry*, :1020-1031.

O'Reilly, E and Pes, L. and Paradisi, F. (2010) 'From amines to diketopiperazines: a one-pot approach'. *Tetrahedron Letters*, 51 :1696-1697.

E. O'Reilly, D. Balducci, **F. Paradisi** "A stereoselective synthesis of  $\alpha$ -deuterium labelled (*S*)- $\alpha$ -amino acids" *Aminoacids* **2010**, 39, 849-858

K. Pandurangan, S. Gallagher, G. G. Morgan, H. Müller-Bunz, **F. Paradisi** "Structure and Anti-Microbial Activity of the Silver(I) Complex of 2-Aminophenoxazine-3-one" *Metallomics* **2010**, 2, 530-534

#### **Dr Andrew Phillips**

Moreno, Aitor; Pregosin, Paul S.; Laurency, Gabor; Phillips, Andrew D.; Dyson, Paul J. (2009) 'Influence of Ion Pairing on Styrene Hydrogenation Using a Cationic h 6-

Arene b -Diketiminato-Ruthenium Complex'. *Organometallics*, 28 (22):6432-6441.



Renfrew, A. K., Phillips, A. D., Egger, A. E., Hartinger, C. G., Bosquain, S. S., Nazarov, A. A., Keppler, B. K., Gonsalvi, L., Peruzzini, M., Dyson, P. J. (2009) 'Influence of Structural Variation on the Anticancer Activity of RAPTA-Type Complexes: ptn versus pta'. *Organometallics*, 28 (4):1165-1172.

#### [Professor Gareth Patrick Redmond](#)

Jang, JI, Mani, S, Ketterson, JB, Lovera, P, Redmond, G (2009) 'Nonlinear refractive index and three-photon absorption coefficient of poly(9,9-dioctylfluorene)'. *Applied Physics Letters*, 95 .

**Dr James Anthony Sullivan**

Sullivan, JA; Flanagan, KA; Hain, H (2009) 'Suzuki coupling activity of an aqueous phase Pd nanoparticle dispersion and a carbon nanotube/Pd nanoparticle composite'. *Catalysis Today*, 145 (1-2):108-113.

James A Sullivan and Petrica Dulgheru (2010) 'The effect of C(s) on the trapping of NOx onto Pt/Ba/Al<sub>2</sub>O<sub>3</sub> catalysts'. *Applied Catalysis B: Environmental*, 99 :235-241. [\[DOI\]](#) [\[Details\]](#)

**Dr Matthias Tacke**

A. Deally, J. Claffey, B. Gleeson, M. Hogan, H. Müller-Bunz, S. Patil, D. O'Shea, M. Tacke (2010) 'Synthesis and Preliminary Cytotoxicity Studies of Achiral Pyrrolyl-Substituted Titanocenes'. *Polyhedron*, 29 (12):2445-2453.

J. Claffey, H. Müller-Bunz, M. Tacke (2010) 'Benzyl-Substituted Titanocene Dichloride Anticancer Drugs: From Lead to Hit'. *Journal of Organometallic Chemistry*, 695 :2105-2117.

M. Hogan, B. Gleeson, M. Tacke (2010) 'The Cytotoxicity of Titanocene Y against CAKI-1 Cells: An In Vitro Formulation Study'. *Letters in Drug Design & Discovery*, 7 (5):310-317.

B. Gleeson, J. Claffey, M. Hogan, H. Müller-Bunz, D. Wallis, M. Tacke (2010) 'Novel Benzyl-Substituted Molybdocene Anticancer Drugs'. *Inorganica Chimica Acta*, 363 :1831-1836.

A. Erxleben, J. Claffey, M. Tacke (2010) 'Binding and hydrolysis studies of antitumoural titanocene dichloride and Titanocene Y with phosphate diesters'. *Journal of Inorganic Biochemistry*, 104 :390-396.

S. Eger, T. A. Immel, J. Claffey, H. Müller-Bunz, M. Tacke, U. Groth, T. Huhn (2010) 'Titanocene difluorides with improved cytotoxic activity'. *Inorganic Chemistry*, 49 :1292-1294.

I. Fichtner, D. Behrens, J. Claffey, A. Deally, B. Gleeson, M. Hogan, H. Weber, M. Tacke (2010) 'Antitumor Activity of Vanadocene Y and its Selenocyanate Derivative in Xenografted CAKI-1 Tumors in Mice'. *Journal of Organometallic Chemistry*, 695 :1175-1181.

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S. Patil, J. Claffey, A. Deally, B. Gleeson, M. Hogan, L. M. Menéndez Méndez, H. Müller-Bunz, F. Paradisi, M. Tacke (2010) 'Synthesis, Cytotoxicity and Antibacterial Studies of p-Methoxybenzyl-Substituted and Benzyl-Substituted N-Heterocyclic Carbene-Silver Complexes'. *European Journal of Inorganic Chemistry*, :1020-1031.

J. Claffey, A. Deally, B. Gleeson, M. Hogan, L. M. Menéndez Méndez, H. Müller-Bunz, D. Wallis, S. Patil, M. Tacke (2009) 'Pseudo-Halide Derivatives of Titanocene Y: Synthesis and Cytotoxicity Studies'. *Metallomics*, 1 :511-517.

#### Dr Xiangming Zhu

Zhong, ZY,Wang, XX,Kong, LC,Zhu, XM (2009) 'Trapping of Isocyanates with Benzotriazole in situ - Preparation of Carbamoyl Benzotriazoles as an Isocyanate Alternative via Curtius Rearrangement'. *Synlett*, :2461-2464.

#### **Dr Susan Quinn**

P. S. Nagle, S. J. Quinn, J. M. Kelly, D. H. O'Donovan, A. R. Khan, F. Rodriguez, B. Nguyen, W. D. Wilson and I. Rozas, (2010) 'Understanding the DNA binding of novel non-symmetrical guanidinium/2-aminoimidazolium derivatives' *Org. Biomol. Chem.*, 2010, **8**, 5558.

S. Vasudevan, J. A. Smith, M. Wojdyla, T. McCabe, N.C. Fletcher, S. J. Quinn and J. M. Kelly (2010) 'Substituted dipyrrophenazine complexes of Cr(III): Synthesis, enantiomeric resolution and binding interactions with calf thymus DNA' *Dalton Trans.*, 2010, **39**, 3990.

S. A. Gallagher, M. P. Moloney, M. Wojdyla, S. J. Quinn, J. M. Kelly and Y. K. Gun'ko (2010) Synthesis and spectroscopic studies of chiral CdSe quantum dots *J. Mater. Chem.*, 2010, 20, 8350-8355.

M. Wojdyla, J.A. Smith, S. Vasudevan, S. J. Quinn, J. M. Kelly (2010) Excited state behaviour of substituted dipyrrophenazine Cr(III) complexes in the presence of nucleic acids *Photochem. Photobiol. Sci.*, 2010, 9, 1196-1202.

#### **Conference Publications**

##### Dr James Anthony Sullivan

Sarah Burnham and James A Sullivan (2010) Oxidation of Glycerol over Titania Supported Gold Catalysts *Japan-UK Symposium: Catalysis for a Sustainable World*,  
E. M. Neville, M. Mattle, J. D. McElroy, M. Rahman B. Rajesh, J. A. Sullivan and K. R. Thampi (2010) Carbon doped TiO<sub>2</sub> through sol-gel processes in the presence of melamine - towards more efficient photocatalysts *Inaugural European Energy Conference*,

M. Jhansi L. Kishore, Kevin Fennell, James A. Sullivan and Grace G. Morgan (2010) Tethering of Cobalt Complexes to Functionalized SBA-15 for Catalytic Fixation of CO<sub>2</sub> *Catalyst Preparation for the 21st Century*,

James A Sullivan (2009) Towards 4-way catalysis *Structure performance relationships at the surface of functional materials*,



Elaine Neville, James A Sullivan (2009) Preparation and characterisation of C-doped TiO<sub>2</sub> photo-catalysts *Europacat IX, Catalysis for a Sustainable World,*

James A Sullivan, Linda Sherry, Petrica Dulgheru, Niamh O'Callaghan (2009) Nano-structured Pd / SBA-15 catalysts for CH<sub>4</sub> combustion and H<sub>2</sub>O<sub>2</sub> production *Europacat IX, Catalysis for a Sustainable World,*

James A Sullivan and Petrica Dulgheru (2009) The effect of using alkali or alkaline earth metal oxides as a NO<sub>x</sub> storage component in a NSR catalyst upon combustion of particulate matter emitted by diesel engines *Europacat IX, Catalysis for a Sustainable World,*

Linda Sherry and James A Sullivan (2009) Tethered Acids and Bases in the Production of FAME *Europacat IX, Catalysis for a Sustainable World,*

