



GlaxoSmithKline

Our ref: COL028898

David Merrifield  
Institute of Particle Science & Engineering  
Houldsworth Building  
Clarendon Road  
University of Leeds  
Leeds  
LS2 9JT

**GlaxoSmithKline Research  
& Development Limited**

Medicines Research Centre  
Gunnels Wood Road  
Stevenage  
Hertfordshire  
SG1 2NY

Tel. +44 (0)1438 745745

Fax. +44 (0)1438 764502

[www.gsk.com](http://www.gsk.com)

15 April 2009

Dear David

**RESEARCH AGREEMENT**

Please find enclosed a copy of the fully executed agreement for your records.

Yours sincerely

Nicky Patrick, PhD  
External Science & Technology

Enc

Registered in England & Wales  
No. 835139

Registered office  
930 Great West Road  
Brentford, Middlesex, TW8 9GS

**THIS AGREEMENT** dated [.....16<sup>th</sup> March.....] 2009 is made **BETWEEN:**

- (1) **THE UNIVERSITY OF LEEDS** whose address is Leeds, LS2 9JT (the University); and
- (2) **GLAXOSMITHKLINE RESEARCH AND DEVELOPMENT LIMITED** whose registered office is at 980 Great West Road, Brentford, Middlesex TW8 9GS, United Kingdom (GSK)

#### **BACKGROUND**

- (A) GSK owns the Equipment (as defined below), which GSK has agreed to loan to the University.
- (B) In consideration for the loan of the Equipment by GSK to the University in support of a PhD project, the University has agreed to grant GSK access to the Results of the Project in accordance with the terms of this Agreement.

#### **1. DEFINITIONS**

In this Agreement the following expressions have the meaning set opposite:

<b>this Agreement:</b>	this document, including its Schedules, as amended from time to time in accordance with clause 11.9;
<b>Background:</b>	information, techniques, Know-how and all other forms of Intellectual Property, software and materials (regardless of the form or medium in which they are disclosed or stored) that are provided by one party to the other for use in the Project (whether before or after the date of this Agreement), except any Result;
<b>a Business Day:</b>	Monday to Friday (inclusive) except bank or public holidays in England;
<b>Confidential Information:</b>	each party's confidential information is: any Background disclosed by that party to the other for use in the Project and identified as confidential before or at the time of disclosure; and any Results in which that party owns the Intellectual Property;
<b>the Effective Date:</b>	16 <sup>th</sup> March 2009
<b>Equipment:</b>	Inverse Gas Chromatography (IGC) System 2 Asset no 062429; Biomax no 209350 – valued at £100,000
<b>Equipment Loan Form:</b>	the agreement governing the loan of Equipment to the University, in the form set out in Schedule 2 to this Agreement;

<b>a Group Company:</b>	any undertaking which is, on or after the date of this Agreement from time to time, a subsidiary undertaking of GSK, a parent undertaking of GSK or a subsidiary undertaking of a parent undertaking of GSK, as those terms are defined in section 258 of the Companies Act 1985 (UK);
<b>Intellectual Property:</b>	patents, trade marks, service marks, registered designs, copyrights, database rights, design rights, confidential information, applications for any of the above, and any similar right recognised from time to time in any jurisdiction, together with all rights of action in relation to the infringement of any of the above;
<b>the Key Personnel:</b>	the Principal Investigator and any other key personnel identified in Schedule 1;
<b>Know-how</b>	unpatented technical information (including, without limitation, information relating to inventions, discoveries, concepts, methodologies, models, research, development and testing procedures, the results of experiments, tests and trials, manufacturing processes, techniques and specifications, quality control data, analyses, reports and submissions) that is not in the public domain;
<b>the Location:</b>	the "Institute of Process Research and Development (IPRD) where the Project will be carried out;
<b>the Principal Investigator:</b>	Professor Kevin Roberts or his successor appointed under clause 10.3;
<b>the Project:</b>	The programme of work described in Schedule 1, as amended from time to time in accordance with clause 11.9;.
<b>the Results:</b>	all information, Know-how, results, inventions, software and other Intellectual Property identified or first reduced to practice or writing in the course of the Project; and
<b>GSK's Supervisor:</b>	Dr Greg Webber or his successor appointed under clause 10.3.

## 2. THE PROJECT

- 2.1 The Project will begin on the Effective Date and will continue until [third anniversary of the Effective Date] or until any later date agreed in writing between the parties, or

until this Agreement is terminated in accordance with clause 8 or 9. If this Agreement is entered into after the Effective Date, it will apply retrospectively to work carried out in relation to the Project on or after the Effective Date.

- 2.2 The University will use reasonable endeavours to carry out the tasks allotted to it in Schedule 1, and will provide the human resources, materials, facilities and equipment that are designated as its responsibility in Schedule 1. The Project will be carried on under the direction and supervision of the Principal Investigator at the Location.
- 2.3 Although the University will use reasonable endeavours to carry out the Project in accordance with Schedule 1, the University does not undertake that any research will lead to any particular result, nor does it guarantee a successful outcome to the Project.
- 2.4 The University will provide GSK with reports summarising the progress of the Project and a copy of all of the Results.
- 2.5 The University warrants to GSK that the University has full power and authority under its constitution, and has taken all necessary actions and obtained all authorisations, licences, consents and approvals, to allow it to enter into this Agreement and to carry out the Project.

### **3. EQUIPMENT TRANSFER**

- 3.1 GSK shall loan the Equipment to the University for the duration of the Project, in return for access to the Results as detailed in clause 4 of this Agreement. The University agree to maintain the Equipment for the duration of the loan in accordance with the Equipment Loan Form.

### **4. USE AND EXPLOITATION OF INTELLECTUAL PROPERTY**

- 4.1 This Agreement does not affect the ownership of any Intellectual Property in any Background or in any other technology, design, work, invention, software, data, technique, Know-how, or materials that are not Results. The Intellectual Property in them will remain the property of the party that contributes them to the Project. No licence to use any Intellectual Property is granted or implied by this Agreement except the rights expressly granted in this Agreement.
- 4.2 The University will own the Intellectual Property in the Results and may take such steps as it may decide from time to time, and at its own expense, to register and maintain any protection for that Intellectual Property, including filing and prosecuting patent applications for any of the Results. Where any third party such as a student or contractor is involved in the Project, the University or the party engaging that contractor (as the case may be) will ensure that that student and that contractor assign any Intellectual Property they may have in the Results in order to be able to give effect to the provisions of this clause 4.
- 4.3 With the exception of any software system which may be developed by Leeds as a result of this Project, the University grants to GSK a non-exclusive, perpetual, fully paid-up, royalty-free licence (with the right to sub-license to any Group Company and to any person working for, or on behalf of, GSK or any Group Company, but only

for the purpose of carrying out that work, and otherwise without the right to sub-license) to use the Intellectual Property in any of the Results for any purpose.

## 5. **ACADEMIC PUBLICATION**

5.1 The Project is undertaken in pursuance of a primary charitable purpose of the University, namely the advancement of education through teaching and research. Therefore, any employee or student of the University (whether or not involved in the Project) may:

- 5.1.1 discuss work undertaken as part of the Project in University seminars, tutorials and lectures; and
- 5.1.2 publish any Background of GSK (unless it is GSK's Confidential Information) or any of the Results.

5.2 GSK will be acknowledged in all such publications or other public disclosures.

## 6. **CONFIDENTIALITY**

6.1 Neither party will, either during the term of this Agreement or for 5 years thereafter, disclose to any third party, nor use for any purpose except carrying out the Project, any of the other party's Confidential Information.

6.2 Neither party will be in breach of any obligation to keep any Background, Results or other information confidential or not to disclose it to any other party to the extent that it:

- 6.2.1 is known to the party making the disclosure before its receipt from the other party, and not already subject to any obligation of confidentiality to the other party;
- 6.2.2 is or becomes publicly known without any breach of this Agreement or any other undertaking to keep it confidential;
- 6.2.3 has been obtained by the party making the disclosure from a third party in circumstances where the party making the disclosure has no reason to believe that there has been a breach of an obligation of confidentiality owed to the other party;
- 6.2.4 has been independently developed by the party making the disclosure;
- 6.2.5 is disclosed pursuant to the requirement of any law or regulation (provided, in the case of a disclosure under the Freedom of Information Act 2000, none of the exceptions to that Act applies to the information disclosed) or the order of any Court of competent jurisdiction, and the party required to make that disclosure has informed the other, within a reasonable time after being required to make the disclosure, of the requirement to make the disclosure and the information required to be disclosed; or
- 6.2.6 is approved for release in writing by an authorised representative of the other party.

6.3 GSK will not be in breach of any obligation to keep any of the Results owned by the University, the University's Background, or other information, confidential or not to disclose them to any third party, by making them available to any Group Company or any person working for or on behalf of GSK or a Group Company, who needs to know the same in order to exercise the rights granted in clause 4.4, provided they

are not used except as expressly permitted by this Agreement and the recipient undertakes to keep that Background, those Results or that information confidential.

- 6.4 If the University receives a request under the Freedom of Information Act 2000 to disclose any information that, under this Agreement, is GSK's Confidential Information, it will notify GSK and will consult with GSK. GSK will respond to the University within 10 days after receiving the University's notice if that notice requests GSK to provide information to assist the University to determine whether or not an exemption to the Freedom of Information Act applies to the information requested under that Act.
- 6.5 Neither the University nor GSK will use the other's name or logo in any press release or product advertising, or for any other promotional purpose, without first obtaining the other's written consent.

## **7. LIMITATION OF LIABILITY**

- 7.1 Neither of the parties makes any representation or gives any warranty to the other that any advice or information given by it or any of its employees or students who work on the Project, or the content or use of any Results, Background or materials, works or information provided in connection with the Project, will not constitute or result in any infringement of third-party rights.
- 7.2 GSK makes no representations or warranties of any kind, that the use of the Equipment will not infringe any patent, copyright, trademark, or other proprietary rights.
- 7.3 Subject to clause 7.6, neither party accepts any responsibility for any use which may be made by the other party of any Results, nor for any reliance which may be placed by that other party on any Results, nor for advice or information given in connection with any Results.
- 7.4 With regard to the Equipment, the University shall defend, indemnify and hold harmless GSK and its Group Companies, and their employees, directors and officers, from and against any and all liabilities, damages, losses or claims for damages to the Equipment or injury to persons diagnosed or injured from use of the Equipment as a result of the provision of the Equipment by GSK during the period of the loan, except to the extent attributable to the negligence or wilful misconduct of GSK or its subsidiaries, and their employees, directors and officers.
- 7.5 Subject to clause 7.6, and except under the indemnity in clause 7.4, the liability of either party to the other for any breach of this Agreement, any negligence, or arising in any other way out of the subject matter of this Agreement, the Project and the Results, will not extend to any indirect damages or losses, or any loss of profits, loss of revenue, loss of data, loss of contracts or opportunity, whether direct or indirect, even if the party bringing the claim has advised the other of the possibility of those losses, or if they were within the other party's contemplation.
- 7.6 Nothing in this Agreement limits or excludes either party's liability for:
- 7.6.1 death or personal injury caused by negligence; or
- 7.6.2 any fraud or for any sort of liability that, by law, cannot be limited or excluded.

7.7 The express undertakings and warranties given by the parties in this Agreement are in lieu of all other warranties, conditions, terms, undertakings and obligations, whether express or implied by statute, common law, custom, trade usage, course of dealing or in any other way. All of these are excluded to the fullest extent permitted by law.

## **8. FORCE MAJEURE**

8.1 If the performance by either party of any of its obligations under this Agreement (except a payment obligation) is delayed or prevented by circumstances beyond its reasonable control, that party will not be in breach of this Agreement because of that delay in performance. However, if the delay in performance is more than 3 months, the other party may terminate this Agreement with immediate effect by giving written notice to the other party.

## **9. TERM AND TERMINATION**

9.1 This Agreement will commence on the Effective Date and will continue until the [third anniversary] of the Effective Date, or until terminated in accordance with clause 8 or 9.

9.2 Either party may terminate this Agreement with immediate effect by giving notice to the other party if:

9.2.1 the other party is in breach of any provision of this Agreement and (if it is capable of remedy) the breach has not been remedied within 60 days after receipt of written notice specifying the breach and requiring its remedy; or

9.2.2 the other party becomes insolvent, or if an order is made or a resolution is passed for its winding up (except voluntarily for the purpose of solvent amalgamation or reconstruction), or if an administrator, administrative receiver or receiver is appointed over the whole or any part of the other party's assets, or if the other party makes any arrangement with its creditors.

9.3 Each of the parties will notify the other promptly if at any time any of the Key Personnel appointed by that party is unable or unwilling to continue to be involved in the Project. Within 3 months after the date of that notice, the party who originally appointed that member of the Key Personnel will nominate a successor. The other party will not unreasonably refuse to accept the nominated successor or if the appointor cannot find a successor, either party may terminate this Agreement by giving the other not less than 3 months' notice.

9.4 Upon termination of the Agreement the University shall return the Equipment to GSK within 60 days of the termination date, unless otherwise agreed in writing.

9.5 Clauses 1, 4, 5, 6, 7, 9.5 and 10 will survive the termination of this Agreement for any reason and will continue indefinitely.

## **10. GENERAL**

10.1 **Notices:** Any notice to be given under this Agreement must be in writing, may be delivered to the other party or parties by any of the methods set out in the left hand



column below, and will be deemed to be received on the corresponding day set out in the right hand column:

<b>Method of service</b>	<b>Deemed day of receipt</b>
By hand or courier	the day of delivery
By pre-paid first class post	the second Business Day after posting
By recorded delivery post	the next Business Day after posting
By fax (provided the sender's fax machine confirms complete and error-free transmission of that notice to the correct fax number)	the next Business Day after sending or, if sent before 16.00 (sender's local time) on the Business Day it was sent

The parties' respective representatives for the receipt of notices are, until changed by notice given in accordance with this clause, as follows:

<b>For the University:</b>	<b>For GSK:</b>
Name:	Name: Dr Nicky Pattrick
Address:	Address: Medicines Research Centre, Gunnels Wood Road, Stevenage, Hertfordshire. SG1 2NY
Fax number:	Fax number: 01438 763276

- 10.2 **Headings:** The headings in this Agreement are for ease of reference only; they do not affect its construction or interpretation.
- 10.3 **Assignment:** Neither party may assign or transfer this Agreement as a whole, or any of its rights or obligations under it, without first obtaining the written consent of the other party. That consent may not be unreasonably withheld or delayed.
- 10.4 **Illegal/unenforceable provisions:** If the whole or any part of any provision of this Agreement is void or unenforceable in any jurisdiction, the other provisions of this Agreement, and the rest of the void or unenforceable provision, will continue in force in that jurisdiction, and the validity and enforceability of that provision in any other jurisdiction will not be affected.
- 10.5 **Waiver of rights:** If a party fails to enforce, or delays in enforcing, an obligation of the other party, or fails to exercise, or delays in exercising, a right under this Agreement, that failure or delay will not affect its right to enforce that obligation or constitute a waiver of that right. Any waiver of any provision of this Agreement will not, unless expressly stated to the contrary, constitute a waiver of that provision on a future occasion.



- 10.6 **No agency:** Nothing in this Agreement creates, implies or evidences any partnership or joint venture between the parties, or the relationship between them of principal and agent. Neither party has any authority to make any representation or commitment, or to incur any liability, on behalf of the other.
- 10.7 **Entire agreement:** This Agreement constitutes the entire agreement between the parties relating to its subject matter. Each party acknowledges that it has not entered into this Agreement on the basis of any warranty, representation, statement, agreement or undertaking except those expressly set out in this Agreement. Each party waives any claim for breach of this Agreement, or any right to rescind this Agreement in respect of, any representation which is not an express provision of this Agreement. However, this clause does not exclude any liability which either party may have to the other (or any right which either party may have to rescind this Agreement) in respect of any fraudulent misrepresentation or fraudulent concealment prior to the execution of this Agreement.
- 10.8 **Further Assurance:** Each party will take any action and execute any document reasonably required by the other party to give effect to any of its rights under this Agreement, or to enable their registration in any relevant territory provided the requesting party pays the other party's reasonable expenses.
- 10.9 **Amendments:** No variation or amendment of this Agreement will be effective unless it is made in writing and signed by each party's representative.
- 10.10 **Third parties:** No one except a party to this Agreement has any right to prevent the amendment of this Agreement or its termination, and no one except a party to this Agreement may enforce any benefit conferred by this Agreement, unless this Agreement expressly provides otherwise.
- 10.11 **Governing law:** This Agreement is governed by, and is to be construed in accordance with, English law. The English Courts will have exclusive jurisdiction to deal with any dispute which has arisen or may arise out of, or in connection with, this Agreement, except that either party may bring proceedings for an injunction in any jurisdiction.
- 10.12 **Escalation:** If the parties are unable to reach agreement on any issue concerning this Agreement or the Project within 14 days after one party has notified the other of that issue, they will refer the matter to the Vice-Chancellor in the case of the University, and to the Vice-President, External Science & Technology in the case of GSK in an attempt to resolve the issue within 14 days after the referral. Either party may bring proceedings in accordance with clause 10.11 if the matter has not been resolved within that 14 day period, and either party may apply to the court for an injunction whether or not any issue has been escalated under this clause.
- 10.13 **Ethical Standards:** Unless otherwise required or prohibited by law, the Parties warrant, to the best of their knowledge, that in relation to the performance of this Agreement:
- 10.13.1 they do not employ engage or otherwise use any child labour in circumstances such that the tasks performed by any such child labour could reasonably be foreseen to cause either physical or emotional impairment to the development of such child;

- 10.13.2 they do not use forced labour in any form (prison, indentured, bonded or otherwise) and its employees are not required to lodge papers or deposits on starting work;
- 10.13.3 they provide a safe and healthy workplace, presenting no immediate hazards to its employees. Any housing provided by the parties to their employees is safe for habitation. The parties provides access to clean water, food, and emergency healthcare to their employees in the event of accidents or incidents in the workplace;
- 10.13.4 they do not discriminate against any employees on any ground (including race, religion, disability or gender);
- 10.13.5 they do not engage in or support the use of corporal punishment, mental, physical, sexual or verbal abuse and does not use cruel or abusive disciplinary practices in the workplace;
- 10.13.6 they pay each employee at least the minimum wage, or a fair representation of the prevailing industry wage, (whichever is the higher) and provides each employee with all legally mandated benefits;
- 10.13.7 they comply with the laws on working hours and employment rights in the countries in which they operate; and
- 10.13.8 they are respectful of their employees right to join and form independent trade unions and freedom of association;
- 10.13.9 they are responsible for controlling their own supply chain and that they shall encourage compliance with ethical standards and human rights by any subsequent supply of goods and services that are used by the parties when performing their obligations under this Agreement; and
- 10.13.10 they have ethical and human rights policies and an appropriate complaints procedure to deal with any breaches of such policies.

**SIGNATURES ON NEXT PAGE**

**SIGNED** for and on behalf of the  
UNIVERSITY OF LEEDS

Name: *MOHAMED POURKASHANIAN*

Position: *HEAD OF SCHOOL*

Signature



Read and understood by the Principal  
Investigator

Signature

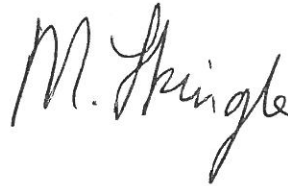
Date

*3.13.09*

**SIGNED** for and on behalf of  
GLAXOSMITHKLINE RESEARCH &  
DEVELOPMENT LIMITED:

Name: **DR MALCOLM SKINGLE**  
**DIRECTOR**  
Position: **EXTERNAL SCIENCE AND**  
**TECHNOLOGY**

Signature



Read and understood by the  
GSK Supervisor

Signature

Date

*G. Webb (G.S. WEBB)*

*8th April 2009*

## SCHEDULE 1

### The Project

#### **Relating the surface characteristics of pharmaceutical powders to their prior processing, by linking IGC measurements with molecular modelling.**

K.J. Roberts, M.Ghadiri and R.B. Hammond, Institute of Particle Science & Engineering (IPSE), School of Process, Environmental and Materials Engineering, University of Leeds, Leeds LS2 9JT

#### **Project Background**

Variability in the end physical properties of crystalline pharmaceutical APIs can have significant impact on downstream formulation e.g. through variation in blending, granulation, drying and compaction properties: in particular variability in API particle size/shape distributions, either due to the crystallisation or milling steps, can have a significant impact. The influence of processing on pre-formulated APIs is often assessed by analytical techniques such as DSC, TGA, DVS and IGC. The latter is particularly useful as, via studies of solvent vapour retention times, the surface energy of the powder can be estimated. However, such measurements only provide a broad indication of surface state, reflecting the fact that surface energy depends on the exposed crystallographic surfaces and these are not only highly system-specific but also can vary during processing, i.e. crystal habit changes during crystallisation and particle fracture during milling. Hence, there is an important need to provide a more molecular-scale understanding of pharmaceutical unit processes and a validation of the associated analytical methodology in order to be able to meet future regulatory needs. The latter, is becoming highly topical with respect to the industry's need, through the requirements of ICHQ8, to be able to register the process design space of future products.

Recent research at IPSE in Leeds have resulted [1-4] in the development of a new molecular modelling tool POLYPACK which enables morphological modelling tools, notably morphological prediction based on API Crystal structure information via the HABIT [5-7] programme, to be extended to produce a molecular model of a faceted particle. From this and incorporating grid-based searching techniques [8-12] a number of useful physical properties can be calculated:

- Surface area/face (like);
- Bulk volume and equivalent diameter;
- Particle dimensions and aspect ratio;
- Surface charge and hydrophobicity / hydrophilicity;
- Cluster structure as a function of particle size;
- Surface roughness, wetting and contact angle;
- Vacuum surface energy and interfacial tension as a function of solvent.

#### **Proposed PhD Study**

The recent developments in modelling capability at Leeds provide, in principle, a route to provide quantitative calculation of surface energetics as a function of particle morphology to compare to IGC data with the aim to provide a computational framework to be able to better understand the influence of processing on surface properties. The validity of this approach has been demonstrated for perfectly faceted crystals through experimental work linked to nucleation studies.

Hence, the proposed PhD programme would aim to examine representative pharmaceutical compounds such as paracetamol,  $\alpha$ -lactose, carbamazepine, aspirin and theophylline. The following research programme is envisaged to:

1. Review the literature on experimental and modelling techniques for characterising particle surface properties. It would focus in particular on iGC techniques, and their application to pharmaceutical materials.
2. Prepare, via defined crystallisation procedures, well-formed faceted examples of these powdered materials. These will be characterised in respect of their particle size distribution; surface area; thermal properties; crystalline structure / polymorphism etc..
3. Characterise the crystal morphology of the material in terms of its crystallographic forms (hkl) and their associated surface areas using the POLYPACK program cited above.
4. Examine the above materials with iGC techniques, using both polar and apolar solvent probes, and calculate the material's net interfacial tension (both dispersive and polar contributions to the intermolecular interactions).
5. Extend grid based search molecular modelling methodology to characterise the interfacial tension of individual crystalline surfaces (hkl) based on the material's known crystal morphology, and through this derive the particle's net interfacial tension. It is intended that this will lead to a refinement and validation of iGC analytical approaches.
6. Use the validated model to determine the interfacial tensions for the crystal surfaces and relate this to the surface chemistry as predicted by molecular modelling.
7. Test the approach by using crystal habit modifiers to vary the relative proportions of different crystalline faces, and crystallise such material for subsequent iGC analysis.
8. Examine crystals following representative secondary processing such as milling, and through careful characterisation of crystal orientation, estimate the particle's interfacial tension based on its contribution from various habit faces, and through this improve the analytical capability of iGC for assessing the effects of pharmaceutical processing.

Assuming success with the above study, the project would then be extended to co-crystals and salts where certain surfaces may be rich in one or other components, thereby having an important influence on its biopharmaceutical properties.

## References

1. Simulation of the energetic stability of faceted L-glutamic acid nano crystalline clusters in relation to their phase stability as a function of crystal size, R B Hammond, K Pencheva and K J Roberts, *Journal of Physical Chemistry B* 109 (2005) 19550-19552
2. A structural-kinetic approach to model face-specific solution/crystal surface energy associated with the crystallisation of acetyl salicylic acid from supersaturated aqueous/ethanol solutions, R B Hammond, K Pencheva and K J Roberts, *Crystal Growth and Design* 6 (2006) 1324-1334

3. Quantifying solubility enhancement due to particle size reduction and crystal habit modification: Case study of acetyl salicylic acid, R B Hammond, K Pencheva, K J Roberts and T Auffret, submitted to Journal of Pharmaceutical Sciences (2006)
4. Molecular modelling of interfacial crystal/crystal interactions between the  $\alpha$ - and  $\beta$ -forms of L-glutamic acid using grid-based methods, R B Hammond, K Pencheva and K J Roberts, Crystal Growth and Design (2006) under review
5. The crystal habit of molecular materials: A structural perspective, G Clydesdale, K J Roberts and E M Walker, In "Molecular Solid State: Syntheses, Structure, Reactions, Applications" Volume 2, "Theoretical Aspects and Computer Modelling" (Ed. A Gavezzotti), chapter 7 (1996), 203-232
6. Modelling the crystal morphology of alkali alkyl surfactants: sodium and rubidium dodecyl sulphates, L A Smith, G B Thomson, K J Roberts, D Machin and G McLeod, Crystal Growth and Design 5 (2005) 2154-2163
7. A molecular modelling study of the crystal morphology of adipic acid and its habit modification by homologous impurities, G Clydesdale, G B Thomson, E M Walker, K J Roberts, P Meenan and R Docherty, Crystal Growth and Design 5 (2005) 2164-2172
8. Computationally assisted structure determination for molecular materials from X-ray powder diffraction data, R B Hammond, K J Roberts, R Docherty and M Edmondson, Journal of Physical Chemistry 101 (1997) 6532-6536
9. Application of systematic search methods to studies of the structures of urea dihydroxy benzene co-crystals, R B Hammond, C Ma, K J Roberts, P Y Ghi, R K Harris, Journal of Physical Chemistry 107 (2003) 11820-11826
10. Grid-based molecular modelling for pharmaceutical salt screening: Case example of 3,4,6,7,8,9-hexahydro-2Hpyrimido (1,2-a) pyrimidinium acetate, R B Hammond, R S Hashim, C Y Ma and K J Roberts, Journal of Pharmaceutical Sciences 95 (2006) 2361-2372
11. Molecular modelling of bulk impurity segregation and impurity-mediated crystal habit modification of naphthalene and phenanthrene in the presence of heterogeneous species, G Clydesdale, R B Hammond and K J Roberts, J Physical Chemistry 107 (2003) 4826-4833
12. Molecular and solid-state modelling of the crystal purity and morphology of  $\epsilon$ -caprolactam in the presence of synthesis impurities and the imino tautomeric species caprolactim, P Mougín, G Clydesdale, R B Hammond and K J Roberts, Journal of Physical Chemistry 107 (2003) 13262-13272

**SCHEDULE 2**  
**EQUIPMENT LOAN FORM**

Professor Kevin Roberts  
School of Process, Environmental and Materials Engineering  
Houldsworth Building  
Clarendon Road  
The University of Leeds  
Leeds  
LS2 9JT

Dear Sirs,

**Loan of Second-hand IGC System 2. Asset no 062429; Biomax no 209350**

The above Equipment is loaned to you on the following conditions:

1. The Equipment is loaned at the University's risk as seen, with all defects and no guarantee as to suitability, capacity, quality, conditions, performance or otherwise is given.
2. The Goods are loaned subject to agreement by the University that it will perform the following: install, commission, use and maintain the Equipment in accordance with the Manufacturer's instructions to ensure that so far as is reasonably practicable it will be safe and without risk to health and be properly used for the purpose for which it is designed.
3. GSK will be responsible for the transfer of the Equipment from GSK's premises to the University. All costs associated with such transfer including appropriate insurance shall be borne by the University. The University acknowledges that it shall be responsible for insuring the Equipment for its replacement value.
4. The University will not remove any GSK labels or other indications of ownership from the Equipment. The University will keep the Equipment securely in its possession at all times and not permit any third party to remove the Equipment from the University's premises without the prior written consent of GSK.

Yours faithfully,  
for GlaxoSmithKline

*G. Webb (G.S. Webb) 8<sup>th</sup> APRIL 2009*

I agree to the loan of this instrument on the above conditions.

For the University of Leeds

Signature:

*M. Pourkashanian*

Name: *MOHAMED POURKASHANIAN*

Date

*30-03-2009.*