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|  |  | **Date:** [02/09/2015] |
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| To: Director Publications  BENTHAM SCIENCE PUBLISHERS LTD  Executive Suite Y-2  PO Box 7917, Saif Zone  Sharjah  UNITED ARAB EMIRATES |
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| Fax: +971-6-557-1134 (UAE)  Email: [benthams@emirates.net.ae](mailto:benthams@emirates.net.ae) / [cad@benthamscience.org](mailto:cad@benthamscience.org) |
|  |

Dear Sir

Re: Copyright assignment and publishing agreement – Subscription Journals

Please find attached a copy of Bentham Science Publishers Ltd’s (“Bentham Science”) *Standard Terms & Conditions*, along with Schedules related to the subject copyright work (the “Work”), namely:

|  |
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| TITLE OF WORK: Prediction of Mutagenicity of Chemicals from Their Calculated Molecular Descriptors: A Case Study with Structurally Homogeneous versus Diverse Datasets |

I am the Principal / Corresponding Author of the Work, and my contact details are found in the signature block below.

In order to submit the Work for publication with Bentham Science, I understand that it is necessary to complete and submit this Copyright Letter, along with the *Standard Terms & Conditions* and the attached Schedules. I further understand that these documents together comprise the copyright assignment and publishing agreement between myself and Bentham Science relating to the Work.

I have signed and dated this Copyright Letter, the *Standard Terms & Conditions*, and the Schedules. Please have these documents countersigned on behalf of Bentham Science, and return a copy to me by email at your nearest opportunity.

Yours faithfully

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| Name:  **Principal / Corresponding Author of the Work (“Assignor”)**  Affiliation:  Address:  Fax: Telephone:  Email 1: Email 2: |

*STANDARD TERMS & CONDITIONS*

1. BACKGROUND
   1. The “Work” is the research article, review article, letter, clinical trial study, report, article, or other copyright work, as identified in the Copyright Letter and further detailed in *Schedule 1: Details of the Work* (including such form of the copyright work submitted to Bentham Science for publication pursuant to clause 4, below), but excluding (except where context otherwise requires) any diagrams, figures or illustration specifically identified to Bentham Science pursuant to clause 3.2, below.
   2. Bentham Science and the Assignor agree that these Standard Terms & Conditions, along with the details set-out in the Copyright Letter and in the Schedules, comprise the agreement between the parties relating to Work (the “Agreement”).
2. AUTHORS
   1. The individual/s identified in *Schedule 2: Authors* are the authors of the Work (“Author/s”). The Assignor represents and warrants that he or she has full right and power to enter into this Agreement, and (where the Assignor is not the sole author) that the Author/s of the Work consent and agree to the terms of this Agreement and have irrevocably granted all rights in the Work to the Assignor for assignment to Bentham Science in accordance with the terms of this Agreement. Upon request from Bentham Science, the Assignor shall at his/her own expense provide written evidence of the same to Bentham Science.
   2. Bentham Science shall use its best efforts to ensure that the Author/s are properly credited for the Work. The Assignor represents and warrants that the Author/s have, to the fullest extent permitted by applicable law, waived or undertaken to refrain from enforcing against Bentham Science, their moral rights in the Work. Upon request from Bentham Science, the Assignor shall at his/her own expense provide written evidence of the same to Bentham Science.
3. Copyright ASSIGNMENT
   1. Subject to clause 3.2, in consideration of the mutual undertakings contained herein, the Assignor hereby assigns to Bentham Science absolutely with full title guarantee the following rights throughout the world:
      1. the entire copyright and all other rights in the nature of copyright subsisting in the Work and in all preliminary drafts or earlier versions of the Work;
      2. all other rights in the Work of whatever nature (but, for the avoidance of doubt, excluding any intellectual property rights in any theory, apparatus or invention expressed in the Work), whether now known or created in the future, to which the Assignor is now, or at any time after the date of this Agreement may be, entitled by virtue of the laws in force in any part of the world ; and
      3. all rights all rights in and to all physical and digital materials of any kind which embody the Work in whole or in part,

together with all related rights and powers arising or accrued, including the right to bring, make, oppose, defend, appeal and obtain relief (and to retain any damages recovered) in respect of any infringement, or any other cause of action arising from ownership, of any of these assigned rights, whether occurring before, on, or after the date of this Agreement.

* 1. To the extent that copyright in any of the diagrams, illustrations or figures incorporated into the Work does not belong to the Assignor, the Assignor undertakes to specifically identify such diagrams, illustrations or figures to Bentham Science, and to procure for Bentham Science such rights as will enable Bentham Science to use (without limitation) such diagrams, illustrations and figures, without restriction, in the course of publishing the Work. Such rights shall be perpetual and irrevocable, and shall extend to the right to sub-license to third parties in a similar manner. Where context requires, references to “Work” in this Agreement shall include references to such diagrams, illustrations or figures.
  2. Bentham Science may charge, assign and/or license the benefit of this Agreement in whole or in part, including (without limitation) any and all rights assigned or licensed to Bentham Science hereunder, and the benefit of any representations, warranties, indemnities and undertakings of the Assignor, to any third party.

1. DELIVERY AND PUBLISHING
   1. Bentham Science offers publishing via a variety of methods. The parties agree that, at a minimum, and subject to the payment of the Fee by the Assignor (as set out in *Schedule 4: Publishing*) and the other terms of this Agreement, the Work shall be published in the manner specified, and on the commercial terms specified, in *Schedule 4: Publishing*.
   2. The Assignor undertakes to provide to Bentham Science, by the deadline specified in *Schedule 1: Details of the Work* (the “Submission Deadline”), an electronic copy of the Work in a high-quality, professionally prepared, production-ready format. The Assignor undertakes to ensure that all pages of the Work so submitted have been proof-read carefully, and that all diagrams, illustrations, figures and captions, are of excellent quality, with regard to both substance and form.
   3. The Assignor represents and warrants that the Work has been prepared in accordance with the relevant Guidelines, and checked for all possible linguistic inconsistencies and errors, including grammar, style and typography, by someone with a high command of the English language and familiarity with academic writing in the English language. (“Guidelines” means the Author Guidelines or Information for Authors available on the Bentham Science website, as well as the Aims & Scope applicable to the relevant Bentham Science publication). Bentham Science’s nominated service provider, Eureka Science, offers English language support services which Assignor may elect to utilise in respect of the Work by completing the applicable box in *Schedule 1: Details of the Work*. The provision of such services by Eureka Science shall be subject to Eureka Science’s prevailing terms and rates relating to such type of optional support.
   4. In the space provided in *Schedule 1: Details of the Work*, the Assignor shall disclose whether or not the Work reports experiments involving humans or animals, and further represents and warrants that his/her responses to the related questions are accurate.
   5. Bentham Science shall be entitled to carry-out such minor amendments or adjustments to the Work as it considers necessary in order to ensure conformity with Bentham Science’s production and presentation requirements. If Bentham Science notifies the Assignor that the Work requires amendments or adjustments beyond what Bentham Science considers to be minor, then the Assignor may opt to either: i. address such issues directly (within a reasonable timeframe specified by Bentham Science), or ii. instruct Bentham Science to address such issues. If the Assignor instructs Bentham Science to address the issues, Bentham Science’s terms and rates relating to this type of optional support shall apply, and Bentham Science shall confirm the likely costs to the Assignor before commencing any such work.
   6. For quality monitoring purposes, Bentham Science will seek a review of the Work by specialists familiar with the subject matter. The Assignor acknowledges and agrees that acceptance of the Work by Bentham Science and publication of the same shall be subject to positive peer review by independent referees. Bentham Science may consult such referees as it considers appropriate, including referees identified by reference to publication records, recommendations of editorial board members, or otherwise. The Assignor may nominate its own referees in the space provided in *Schedule 3: Proposed Referees*. If the Assignor wishes to nominate referees in this manner, it shall ensure that such referees have not published with the Author/s within the five year period up to the date of this Agreement, and are not affiliated in any way with the Author/s, including without limitation, with the current employer of the Author/s. In no event shall Bentham Science be obliged to consult any referees nominated by the Assignor.
   7. Nothing in this Agreement shall restrict Bentham Science’s ability, as assignee of the copyright in the Work, to publish and market the Work in any manner (including via third parties such as third party aggregators). Bentham Science reserves the right to refrain from publishing the Work, or to withdraw the Work from circulation following publication, at its own discretion. Without limitation, Bentham Science may exercise this right if it determines that the Work contains language errors that exceed 5% or more of the total Work (based on total word count), if the work fails to conform with Bentham Science’s production and presentation requirements, if the work attracts undesirable or negative publicity that Bentham considers may impact on the reputations of the Author/s or Bentham Science, and/or for its own commercial reasons.
2. SELF-ARCHIVING POLICIES

By signing the Copyright Letter the authors retain the rights of self-archiving. Following are the important features of self-archiving policy of Bentham Science journals:

1. Authors can deposit the first draft of a submitted article on their personal websites, their institution’s repositories or any non-commercial repository for personal use, internal institutional use or for permitted scholarly posting only.
2. Authors may deposit the ACCEPTED VERSION of the peer-reviewed article on their personal websites, their institution’s repository or any non-commercial repository such as PMC, arXiv after **12 MONTHS of publication** on the journal website. In addition, an acknowledgement must be given to the original source of publication and a link should be inserted to the published article on the journal's/publisher’s website.
3. If the research is funded by NIH, Wellcome Trust or any other Open Access Mandate, authors are allowed the archiving of published version of manuscripts in an institutional repository after the mandatory embargo period. Authors should first contact the Editorial Office of the journal for information about depositing a copy of the manuscript to a repository. Consistent with the copyright agreement, Bentham Science does not allow archiving of FINAL PUBLISHED VERSION of manuscripts unless under an open access mandate as above.
4. The link to the original source of publication should be provided by inserting the DOI number of the article in the following sentence: “The published manuscript is available at EurekaSelect via <http://www.eurekaselect.com/>[insert DOI].”
5. There is no embargo on the archiving of articles published under the *OPEN ACCESS PLUS* category. Authors are allowed deposition of such articles on institutional, non-commercial repositories and personal websites immediately after publication on the journal website.
6. CONFLICTS

The Assignor shall disclose, in *Schedule 1: Details of the Work*, details relating to all actual or potential conflicts of interest relating to the Work, and all financial contributions relevant to the Work and its publication pursuant to this Agreement. If requested by Bentham Science, the Assignor shall provide Bentham Science with any further information it may request in respect of such matters.

1. WARRANTIES

The Assignor warrants and undertakes that, as at the date of this Agreement:

* + 1. the Work does not contain any plagiarism; the Work is the original work of the Author/s, and has not been copied wholly or substantially from any other work or material or any other source;
    2. the Assignor is the sole legal and beneficial owner of the rights purported to be assigned pursuant to this Agreement, and (if applicable) the Assignor has obtained any and all necessary assignments or other permissions from co-authors and/or employers to ensure that the Assignor is able to comply with its obligations and to assign the rights purported to be assigned pursuant to this Agreement;
    3. the Assignor is exclusively entitled to give all warranties, indemnities, assurances, confirmations, waivers and agreements set out in this Agreement;
    4. the Work has not been published by any third party, or submitted to any third party for consideration for publication, and will not be published by any third party or submitted to any third party for consideration by or on behalf of the Assignor or any of the Author/s;
    5. once the Work has been submitted to Bentham Science for publication in accordance with clause 4, the Assignor will not attempt to withdraw the Work from publication;
    6. the Assignor has not assigned or granted to any third party any of the rights assigned or granted pursuant to this Agreement;
    7. the exploitation of the rights assigned or granted by this Agreement will not infringe the rights of any third party, including without limitation, any third party intellectual property rights and any rights to register the same;
    8. the Assignor is unaware of any infringement, or likely infringement, of any of the rights assigned or granted pursuant to this Agreement;
    9. the rights assigned by this Agreement are free from any security interest, option, mortgage, charge or lien;
    10. the Work is factually accurate and contains no matter which is scandalous, libellous, unlawful, or otherwise actionable;
    11. there are no actual or potential conflicts of interest, except as specified in *Schedule 1: Details of the Work*; and
    12. there has been no financial contribution to the Work, except as specified in *Schedule 1: Details of the Work*.

1. indemnities
   1. The Assignor shall indemnify Bentham Science against all liabilities, costs, expenses, damages and losses (including any direct, indirect or consequential losses, loss of profit, loss of reputation and all interest, penalties and legal costs (calculated on a full indemnity basis) and all other professional costs and expenses) suffered or incurred by Bentham Science arising out of or in connection with:
      1. any breach by the Assignor of any of the warranties contained in clause 7; and
      2. the enforcement of this Agreement.
   2. At the request of Bentham Science, and at the Assignor's own expense, the Assignor shall provide all reasonable assistance to enable Bentham Science to resist any claim, action or proceedings brought against Bentham Science as a consequence of any breach by the Assignor of the warranties contained in clause 7. This indemnity shall apply whether or not Bentham Science has been negligent or at fault.
2. Further assurance
   1. At its own expense the Assignor shall, and shall use all reasonable endeavours to procure that any necessary third party shall, promptly execute such documents and perform such acts as may reasonably be required for the purpose of giving full effect to this Agreement, including assisting Bentham Science in obtaining, defending and enforcing the copyright, and assisting with any other proceedings which may be brought by or against Bentham Science against or by any third party relating to the rights assigned by this Agreement.
   2. The Assignor irrevocably appoints Bentham Science to be its attorney in its name and on its behalf to execute documents, use the Assignor’s name and do all things which are necessary or desirable for Bentham Science to obtain for itself or its nominee the full benefit of this Agreement. This power of attorney is irrevocable as long as any of the Assignor's obligations under this Agreement remain undischarged. The attorney may, in any way it thinks fit and in the name and on behalf of the Assignor:
      1. take any action that this Agreement requires the Assignor to take;
      2. exercise any rights which this Agreement gives to the Assignor; and
      3. appoint and remove one or more substitute attorneys with full power as the Assignor's attorney on terms that the attorney thinks fit.

The Assignor must ratify and confirm everything that the attorney and any substitute attorney does or arranges using the powers granted under this clause.

1. General terms
   1. **Entire agreement:** This Agreement constitutes the entire agreement between the parties and supersedes and extinguishes all previous agreements, promises, assurances, warranties, representations and understandings between them, whether written or oral, relating to its subject matter. Each party agrees that it shall have no remedies in respect of any statement, representation, assurance or warranty (whether made innocently or negligently) that are not set out in this Agreement. Each party agrees that it shall have no claim for innocent or negligent misrepresentation or negligent misstatement based on any statement in this Agreement.
   2. **Confidentiality**: Each party undertakes that it will not at any time hereafter use, divulge or communicate to any person, except to its professional representatives or advisers or as may be required by law or any legal or regulatory authority, any confidential information concerning the business or affairs of the other party which may have or may in future come to its knowledge and each of the parties shall use its reasonable endeavours to prevent the publication or disclosure of any confidential information concerning such matters.
   3. **Waiver:** No failure or delay by a party to exercise any right or remedy provided under this Agreement or by law shall constitute a waiver of that or any other right or remedy, nor shall it prevent or restrict the further exercise of that or any other right or remedy. No single or partial exercise of such right or remedy shall prevent or restrict the further exercise of that or any other right or remedy.
   4. **Variation:** No variation of this Agreement shall be effective unless it is in writing and signed by the parties (or their authorised representatives).
   5. **Severance:** If any provision or part-provision of this Agreement is or becomes invalid, illegal or unenforceable, it shall be deemed modified to the minimum extent necessary to make it valid, legal and enforceable. If such modification is not possible, the relevant provision or part-provision shall be deemed deleted. Any modification to or deletion of a provision or part-provision under this clause shall not affect the validity and enforceability of the rest of this Agreement. If any provision or part-provision of this Agreement is invalid, illegal or unenforceable, the parties shall negotiate in good faith to amend such provision so that, as amended, it is legal, valid and enforceable, and, to the greatest extent possible, achieves the intended commercial result of the original provision.
   6. **Governing law and jurisdiction:** This Agreement and any dispute or claim arising out of or in connection with it or its subject matter or formation (including non-contractual disputes or claims) shall be governed by and construed in accordance with the law of the United Arab Emirates as applied in the Emirate of Dubai. Each party irrevocably agrees that the courts of the Emirate of Dubai shall have non-exclusive jurisdiction to settle any dispute or claim arising out of or in connection with this Agreement or its subject matter or formation (including non-contractual disputes or claims).

We agree to the terms as set out in the Agreement.

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| Signed by:  (signature)  (print name)  **PRINCIPAL/AUTHOR** | Signed by:  \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ (signature)  \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ (print name)  For and on behalf of **BENTHAM SCIENCE PUBLISHERS LTD** |

**SCHEDULE 1: DETAILS OF THE WORK**

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| **TITLE OF WORK:** Prediction of Mutagenicity of Chemicals from Their Calculated Molecular Descriptors: A Case Study with Structurally Homogeneous versus Diverse Datasets |
| **TYPE OF WORK** (select one):  **Review Article Research Article**  **Article Report Letter**  **Clinical Trial Study**  **Other - specify:** |
| **DESCRIPTION OF WORK:** Variation in high-dimensional data is often caused by a few latent factors, and hence dimension reduction or variable selection techniques are often useful in gathering useful information from the data. In this paper we consider two such recent methods: Interrelated two-way clustering and envelope models. We couple these methods with traditional statistical procedures like ridge regression and linear discriminant analysis, and apply them on two data sets which have more predictors than samples (i.e. *n* << *p* scenario) and have several types of molecular descriptors. One of these datasets consists of a congeneric group of Amines while the other has a much diverse collection compounds. The difference of prediction results between these two datasets for both the methods supports the hypothesis that for a congeneric set of compounds, descriptors of a certain type are enough to provide good QSAR models, but as the data set grows diverse including a variety of descriptors can improve model quality considerably. |
| **SUBMISSION DEADLINE:** [INSERT] |
| **APPROXIMATE SPECIFICATIONS:** [ ] words; [ 7 ] pages; [ 1 ] images/drawings/figures |
| We would be grateful if you could please indicate below if your submission is likely to be of particular interest to the pharmaceutical or biotechnology companies.  **[X] YES [ ] NO** |
| **DISCLOSURE REGARDING ACTUAL OR POTENTIAL CONFLICTS OF INTEREST:**  None. |
| **DISCLOSURE REGARDING THIRD PARTY FINANCIAL CONTRIBUTIONS:**  During the work, research of SM was partially supported by the NSF grant IIS-1029711. |
| **LANGUAGE AND EDITING:**  Assignor requires assistance in having the English grammar and style of the Work checked and improved by Bentham Science:  **[ ] YES [X] NO**  If Yes, Eureka Science will provide a quote in respect of the same. |

**SCHEDULE 2: AUTHORS (include Principal/Corresponding and Co-Authors details)**

|  |
| --- |
| **NAME:** Subhash C. Basak  **AFFILIATION:** University of Minnesota Duluth  **EMAIL:** sbasak@nrri.umn.edu  **NAME:** Subhabrata Majumdar  **AFFILIATION:** University of Minnesota Twin Cities  **EMAIL:** majum010@umn.edu  **NAME:**  **AFFILIATION:**  **EMAIL:**  **NAME:**  **AFFILIATION:**  **EMAIL:**  **NAME:**  **AFFILIATION:**  **EMAIL:**  **NAME:**  **AFFILIATION:**  **EMAIL:**  **NAME:**  **AFFILIATION:**  **EMAIL:** |

**SCHEDULE 3: PROPOSED REFEREES**

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| **NAME:**  **AFFILIATION:**  **EMAIL:**  **NAME:**  **AFFILIATION:**  **EMAIL:**  **NAME:**  **AFFILIATION:**  **EMAIL:**  **NAME:**  **AFFILIATION:**  **EMAIL:** |

**SCHEDULE 4: PUBLISHING**

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| **PUBLICATION VIA JOURNAL** | |
| TITLE OF JOURNAL(S): | **Current Computer Aided-Drug Design**  Distributed via [print / online / print and online] (select) |
| “Fee”: | [INSERT] payable in respect of the publication by Bentham Science of the Work via the above journal(s) in accordance with the terms below.  The Assignor may elect to require Bentham Science to make the Work available on an “open access” basis via e-journal publication for all to view and download subject to the payment of a one-off fee of **US 1390** and provided that Bentham Science shall remain exclusively entitled to exploit the Work on a commercial basis as Bentham Science deems fit, acting in its sole discretion.  Assignor hereby requests such “open access” publication and agrees to pay the applicable Fee in accordance with the terms below:  **[ ] YES [X] NO** |
| PAYMENT TERMS: | 1. Bentham Science shall invoice the Assignor in respect of the Fee. The Assignor shall pay the Fee to Bentham Science within 15 days of the date of invoice by means of cheque made payable to “Bentham Science Publishers Ltd”, or by credit card payment (in which case Assignor to complete attached form), or by bank wire transfer to the following bank account:   Bank: Emirates NBD Bank (PJSC), Dubai Main Branch, P.O. Box 2923, Dubai, United Arab  Emirates  Swift Code: EBILAEAD  Account Name: 0511230714903  IBAN AE690260000511230714903   1. The Fee shall be paid in full without any deduction or withholding other than as required by law and the Assignor shall not be entitled to assert any credit, set-off, deduction, counterclaim or abatement of any nature whatsoever against Bentham Science in order to justify withholding payment of any such amount in whole or in part. If the Assignor is required, pursuant to any applicable present or future law, rule or regulation of any competent governmental or other administrative body, to make any deduction or withholding from any amount payable to Bentham Science pursuant to this Agreement, the Assignor shall pay to Bentham Science an additional amount as will, after the deduction or withholding has been made, leave Bentham Science with the same amount as it would have been entitled to receive in the absence of any such requirement to make a deduction or withholding; promptly pay to the relevant authority the amount of such deduction or withholding; and provide evidence of the same to Bentham Science on request. |