# AIMMS publication report for: 2020-11-29

### New papers: 2020-10/11

Punt, A., Bouwmeester, H., Blaauboer, B. J., Coecke, S., Hakkert, B., Hendriks, D. F. G., Jennings, P., Kramer, N. I., Neuhoff, S., Masereeuw, R., Paini, A., Peijnenburg, A. A. C. M., Rooseboom, M., Shuler, M. L., Sorrell, I., Spee, B., Strikwold, M., Van der Meer, A. D., Van der Zande, M., Vinken, M., Yang, H., Bos, P. M. J., Heringa, M. B. **New approach methodologies (NAMs) for human-relevant biokinetics predictions: Meeting the paradigm shift in toxicology towards an animal-free chemical risk assessment** (Altex, 20 Oct 2020)[https://doi.org/10.14573/altex.2003242]

Amir, A., Charalampopoulos, P., Pissis, S. P., Radoszewski, J. **Dynamic and Internal Longest Common Substring** (Algorithmica, 1 Dec 2020)[https://doi.org/10.1007/s00453-020-00744-0]

Xie, C., Slagboom, J., Albulescu, L. O., Somsen, G. W., Vonk, F. J., Casewell, N. R., Kool, J. **Neutralising effects of small molecule toxin inhibitors on nanofractionated coagulopathic Crotalinae snake venoms** (Acta Pharmaceutica Sinica B, Oct 2020)[https://doi.org/10.1016/j.apsb.2020.09.005]

Nugroho, A. D. W., Kleerebezem, M., Bachmann, H. **A Novel Method for Long-Term Analysis of Lactic Acid and Ammonium Production in Non-growing Lactococcus lactis Reveals Pre-culture and Strain Dependence** (Frontiers in Bioengineering and Biotechnology, Oct 2020)[https://doi.org/10.3389/fbioe.2020.580090]

Romasanta, A. K. S., van der Sijde, P., van Muijlwijk-Koezen, J. **Innovation in pharmaceutical R&D: mapping the research landscape** (None, 10 Oct 2020)[https://doi.org/10.1007/s11192-020-03707-y]

Collet, J. W., Roose, T. R., Weijers, B., Maes, B. U., Ruijter, E., Orru, R. V. **Recent Advances in Palladium-Catalyzed Isocyanide Insertions** (Molecules (Basel, Switzerland), 23 Oct 2020)[https://doi.org/10.3390/molecules25214906]

N. Kolodkin, A., Sharma, R. P., Colangelo, A. M., Ignatenko, A., Martorana, F., Jennen, D., Briedé, J. J., Brady, N., Barberis, M., Mondeel, T. D., Papa, M., Kumar, V., Peters, B., Skupin, A., Alberghina, L., Balling, R., Westerhoff, H. V. **ROS networks: designs, aging, Parkinson’s disease and precision therapies** (NPJ systems biology and applications, 1 Dec 2020)[https://doi.org/10.1038/s41540-020-00150-w]

Guzman, L., Besa, G., Linares, D., González, L., Pont, C., Bartolini, M., Haigis, A. C., Legradi, J., Muñoz-Torrero, D., Gómez-Catalán, J., Barenys, M. **Evaluation of the effects of acetylcholinesterase inhibitors in the zebrafish touch-evoked response: quantitative vs. qualitative assessment** (Environmental Sciences Europe, 1 Dec 2020)[https://doi.org/10.1186/s12302-020-00421-7]

Abedin, P., Ganguly, A., Pissis, S. P., Thankachan, S. V. **Efficient data structures for range shortest unique substring queries†Let T[1, n] be a string of length n and T[i, j] be the substring of T starting at position i and ending at position j. A substring T[i, j] of T is a repeat if it occurs more than once in T; otherwise, it is a unique substring of T. Repeats and unique substrings are of great interest in computational biology and information retrieval. Given string T as input, the Shortest Unique Substring problem is to find a shortest substring of T that does not occur elsewhere in T. In this paper, we introduce the range variant of this problem, which we call the Range Shortest Unique Substring problem. The task is to construct a data structure over T answering the following type of online queries efficiently. Given a range [α, β], return a shortest substring T[i, j] of T with exactly one occurrence in [α, β]. We present an O(n log n)-word data structure with O(logw n) query time, where w = Ω(log n) is the word size. Our construction is based on a non-trivial reduction allowing for us to apply a recently introduced optimal geometric data structure [Chan et al., ICALP 2018]. Additionally, we present an O(n)-word data structure with O(√ n logɛ n) query time, where ɛ > 0 is an arbitrarily small constant. The latter data structure relies heavily on another geometric data structure [Nekrich and Navarro, SWAT 2012].General information** (Algorithms, Nov 2020)[https://doi.org/10.3390/a13110276]

Hamilton, D. J., Ábrányi-Balogh, P., Keeley, A., Petri, L., Hrast, M., Imre, T., Wijtmans, M., Gobec, S., de Esch, I. J., Keserű, G. M. **Bromo-cyclobutenaminones as new covalent udp-n-acetylglucosamine enolpyruvyl transferase (Mura) inhibitors** (Pharmaceuticals, Nov 2020)[https://doi.org/10.3390/ph13110362]

Steenhuis, M., Ten Hagen-Jongman, C. M., van Ulsen, P., Luirink, J. **Stress-based high-throughput screening assays to identify inhibitors of cell envelope biogenesis** (Antibiotics, Nov 2020)[https://doi.org/10.3390/antibiotics9110808]

Blankesteijn, M., Bossink, B. **Assessing the Legitimacy of Technological Innovation in the Public Sphere: Recovering Raw Materials from Waste Water This paper researches legitimacy creation in a publicly-funded trajectory of innovative technological development. It develops a framework of input, throughput and output legitimacy. The framework is developed based on a review of the literature on the creation of legitimacy in innovative technological development. The framework assists in further exploring the potential of the integrated assessment of the legitimacy of technological innovation trajectories in the public sphere, in terms of (1) public accountability (ensuring input legitimacy); (2) science, technology and innovation policy (ensuring throughput legitimacy); and (3) the potential for the implementation of the technology itself in practical contexts (ensuring output legitimacy). The framework is used to analyze a case study about the publicly-funded development of innovative technology for the retrieval of raw materials from waste water. Theoretically, the value of a more processual approach to the conceptualization of legitimacy becomes apparent. Furthermore, the framework assists in the development of practical recommendations on the ways in which to optimize the legitimacy in an earlier stage in the innovation’s trajectory. However, due attention should also be paid to the role of regulatory arrangements in the optimization of the legitimacy of publicly-funded technological innovation. This is an avenue for further research.General information** (Sustainability, 12 Nov 2020)[https://doi.org/https://doi.org/10.3390/su1222940810.3390/su12229408]

### New papers: 2020

Landa, I., Westbroek, H., Janssen, F., van Muijlwijk, J., Meeter, M. **Scientific Perspectivism in Secondary-School Chemistry Education: Integrating Concepts and Skills in Chemical Thinking** (Science and Education, 1 Oct 2020)[https://doi.org/10.1007/s11191-020-00145-3]

Romasanta, A. K., van der Sijde, P., van Muijlwijk-Koezen, J. E. **Innovation in pharmaceutical R&D: mapping the research landscape** (None, 10 Oct 2020)[https://doi.org/https://doi.org/10.1007/s11192-020-03707-y]

Bugatti, K., Bruno, A., Arosio, D., Sartori, A., Curti, C., Augustijn, L., Zanardi, F., Battistini, L. **Shifting Towards αVβ6 Integrin Ligands Using Novel Aminoproline-Based Cyclic Peptidomimetics** (Chemistry - A European Journal, 21 Oct 2020)[https://doi.org/10.1002/chem.202002554]

Salvito, D., Fernandez, M., Jenner, K., Lyon, D. Y., de Knecht, J., Mayer, P., MacLeod, M., Eisenreich, K., Leonards, P., Cesnaitis, R., León-Paumen, M., Embry, M., Déglin, S. E. **Improving the Environmental Risk Assessment of Substances of Unknown or Variable Composition, Complex Reaction Products, or Biological Materials** (Environmental toxicology and chemistry, 1 Nov 2020)[https://doi.org/10.1002/etc.4846]

van Beek, L. F., Surmann, K., van den Berg van Saparoea, H. B., Houben, D., Jong, W. S., Hentschker, C., Ederveen, T. H., Mitsi, E., Ferreira, D. M., van Opzeeland, F., van der Gaast–de Jongh, C. E., Joosten, I., Völker, U., Schmidt, F., Luirink, J., Diavatopoulos, D. A., de Jonge, M. I. **Exploring metal availability in the natural niche of Streptococcus pneumoniae to discover potential vaccine antigens** (Virulence, 5 Oct 2020)[https://doi.org/10.1080/21505594.2020.1825908]

Marino, S. D., Gerolin, A. **An Optimal Transport Approach for the Schrödinger Bridge Problem and Convergence of Sinkhorn Algorithm** (Journal of Scientific Computing, 1 Nov 2020)[https://doi.org/10.1007/s10915-020-01325-7]

Adihou, H., Gopalakrishnan, R., Förster, T., Guéret, S. M., Gasper, R., Geschwindner, S., Carrillo García, C., Karatas, H., Pobbati, A. V., Vazquez‐Chantada, M., Davey, P., Wassvik, C. M., Pang, J. K. S., Soh, B. S., Hong, W., Chiarparin, E., Schade, D., Plowright, A. T., Valeur, E., Lemurell, M., Grossmann, T. N., Waldmann, H. **A protein tertiary structure mimetic modulator of the Hippo signalling pathway** (Nature Communications, 1 Nov 2020)[https://doi.org/10.1038/s41467-020-19224-8]

Grimmel, S. A., Teodoro, T. Q., Visscher, L. **Is it worthwhile to go beyond the local-density approximation in subsystem density functional theory?** (International Journal of Quantum Chemistry, 1 Nov 2020)[https://doi.org/10.1002/qua.26111]