**Exploring the structure-property relationship of explosives: the cheminformatics approach**

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**ABSTRACT**

The widespread applications of energetic materials render the need for the accurate assessment of their properties, essential [1]. Their use or storage, demand the knowledge of a wide range of parameters that would help estimating i.e. their performance, impact, shock or friction sensitivity, stability, bioaccumulation etc. Cheminformatics can greatly contribute towards this direction as it offers methods and approaches for the *in silico* evaluation of such properties for a wide range of chemical structures, in minimum cost and time required [2]. Predictive modeling based on the structural characteristics of the compounds for a fast and accurate prediction of the energetic materials properties has been proposed in the literature [3]. This approach allows the virtual high-throughput screening of novel energetic materials not yet synthesized or tested. In this work several examples for the development of *in silico* models for the prediction of critical properties for explosives are first presented. Then specific cheminformatics workflows based on machine learning and artificial intelligence methodologies are developed and proposed to virtually screen novel or non-tested materials [4].

**KEYWORDS:** Cheminformatics, Molecular Descriptors, energetic materials, Machine Learning

**REFERENCES**

[1] Elton DC, et al. (2018) Scientific Reports, 8:9059

[2] Muratov EN, et al. (2020) Chem. Soc. Rev., 49: 3525

[3] Prana V, Fayet G, Routureau P, Adamo C. (2012) J Hazard Mater., 235: 169.

[4] Papadopoulou D, et al. (2021) Int. J. Mol. Sci., 22(19): 10220.