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## **ChemicalToolBoX and its application on the study of the drug like and purchasable space**

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*Published in:*  
Journal of Cheminformatics

*DOI:*  
[10.1186/1758-2946-6-S1-P51](https://doi.org/10.1186/1758-2946-6-S1-P51)

*Publication date:*  
2014

*Licence:*  
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*Document Version*  
Publisher's PDF, also known as Version of record

[Link to publication in Discovery Research Portal](#)

*Citation for published version (APA):*  
Lucas, X., Grüning, B. A., & Günther, S. (2014). ChemicalToolBoX and its application on the study of the drug like and purchasable space. *Journal of Cheminformatics*, 6(Suppl. 1), Article P51. <https://doi.org/10.1186/1758-2946-6-S1-P51>

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POSTER PRESENTATION

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# ChemicalToolBoX and its application on the study of the drug like and purchasable space

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From 9th German Conference on Chemoinformatics  
Fulda, Germany. 10-12 November 2013

The ever increasing amount of data and computational capabilities in the cheminformatics field has led to a scenario where efficient techniques for storage and processing in an integrated, modular, and easily accessible platform are in vital demand. Here, we present ChemicalToolBoX, a compilation of more than 30 tools integrated into a single computational chemistry and cheminformatics platform based on the Galaxy workflow management system [1,2]. We have recently designed a workflow within the ChemicalToolBoX to generate a library of compounds containing around 70 million unique commercially available small molecules, i.e. the purchasable space [3]. Subsequently, we have used filtering rules based on structural patterns and chemical alarms to discard problematic molecules, representing a very large portion of the drug-like and purchasable space, along with other drug discovery data sets including more than 2 million fragments (Figure 1). Furthermore, we have

computed several physicochemical descriptors to discover general trends applying to each subset.

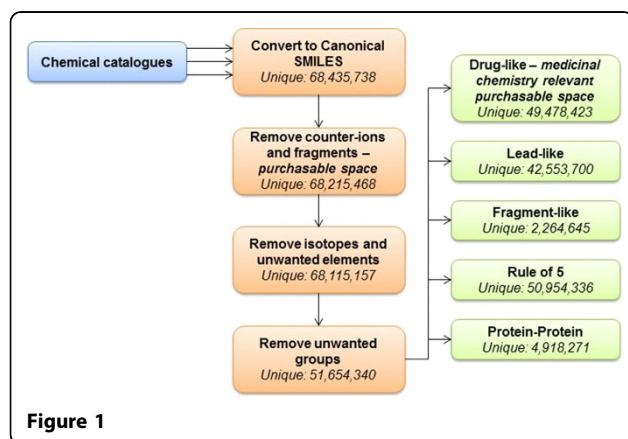
Published: 11 March 2014

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2. Grüning BA, *et al.*, submitted.
3. Lucas X, *et al.*, manuscript in preparation.

doi:10.1186/1758-2946-6-S1-P51

Cite this article as: Lucas *et al.*: ChemicalToolBoX and its application on the study of the drug like and purchasable space. *Journal of Cheminformatics* 2014 **6**(Suppl 1):P51.



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