UABDIVULGA
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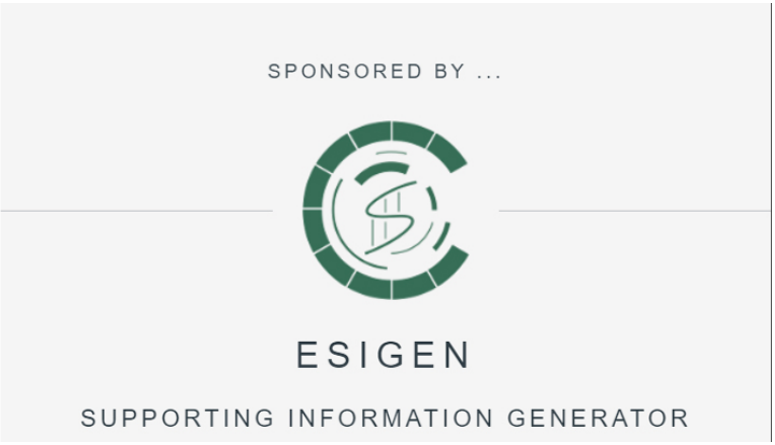
Easily reproducible computational chemistry thanks to ESIgen



ESIgen is a web application that allows to create computational chemistry job reports in an fully automated way. Through its multiple templates, Supporting Information documents can be automagically generated, as well as technical reports suitable for internal communication during the research process.

The application can be tested for free on http://esi.insilichem.com.

Scientific progress is tightly linked to a constant verification of results. Without the validation of other researchers, any advance or achievement is as well as nothing. That is the reason why any scientific communication must be accompanied by the data needed for the reproduction of the research.

However, a work full of technical details can soon become an unreadable text. As a workaround, most of that data is usually collected in a separate document called "Supporting Information".

Even among the most meticulous researchers, collecting all this data results in a tedious work that requires many hours. In computational chemistry, it involves going through tens of files while searching for the adequate values, only to have them copied and pasted in text processor. It is a work that must be done, but it is painfully inefficient. Fortunately, all that labour can be reduced to a series of repetitive actions easily automatizable with the aid of programming languages.

ESIgen is a tool conceived to alleviate the creation of Supporting Information documents in computational chemistry, The user only needs to drag and drop the pertinent files in the web interface, letting the server do the hard work: it will extract and present the relevant information in a fully automated way. The resulting document can be exported to scientific data storage services like FigShare or Zenodo, or downloaded to the hard drive. The file formats available put an emphasis in reproducible data, easily importable in scientific software, although ready-to-print PDF documents are also available.

Advanced users can benefit from batch processing thanks to the command-line interface or Python scripting. All the source code is freely available at GitHub.

Jaime Rodríguez-Guerra
Chemistry Department
Physical Chemistry Area
Universitat Autònoma de Barcelona
jaime.rodriguezguerra@uab.cat

References

Jaime Rodríguez Guerra Pedregal, Pablo Gómez-Orellana, Jean Didier Maréchal**. ESIgen: Electronic Supporting Information Generator for Computational Chemistry Publications***. J. Chem. Inf. Model., 2018, 58 (3), pp 561–564*

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