

Modern visualization of partial atomic charges in Mol*

Bachelor's thesis defense

Dominik Tichý

492772@mail.muni.cz

Faculty of Informatics, Masaryk University

June 15, 2023

Frame Title

Frame Subtitle

plain text, [page structure](#), emphasis

- a single-line bullet list item
- a bullet list item that is quite long (in order to force a line break), which also contains emphasized text
 - a second-level list item
 - a third-level list item
 - an emphasized second-level list item
- 1. a numbered list item
 - 1.1 a second-level list item containing a math expression

$$E = mc^2$$

and a citation

Text Blocks

text above a block¹

Block

text in a block

Example Block

text in a block

Emphasized Block

text in a block

¹a footnote with an <https://address.edu>

Contribution of the thesis

NAR paper

JOURNAL ARTICLE

α Charges: partial atomic charges for AlphaFold structures in high quality

Ondřej Schindler, Karel Berka, Alessio Cantara, Aleš Křenek, Dominik Tichý,
Tomáš Raček , Radka Svobodová 

Nucleic Acids Research, gkad349, <https://doi.org/10.1093/nar/gkad349>

Published: 09 May 2023 **Article history** ▼

Figure: NAR paper [1]

Conclusion

- created a visualization of partial atomic charges in Mol*
- integrated the visualization into the ACC2 and α Charges web applications
- extended the capabilities of the ACC2 web application
- contributed with the work to the NAR paper

Bibliography I

- [1] Ondřej Schindler et al. “ α Charges: partial atomic charges for AlphaFold structures in high quality”. In: *Nucleic Acids Research* (May 2023). gkad349. ISSN: 0305-1048. DOI: 10.1093/nar/gkad349. eprint: <https://academic.oup.com/nar/advance-article-pdf/doi/10.1093/nar/gkad349/50252244/gkad349.pdf>. URL: <https://doi.org/10.1093/nar/gkad349>.

MUNI

FACULTY

OF INFORMATICS